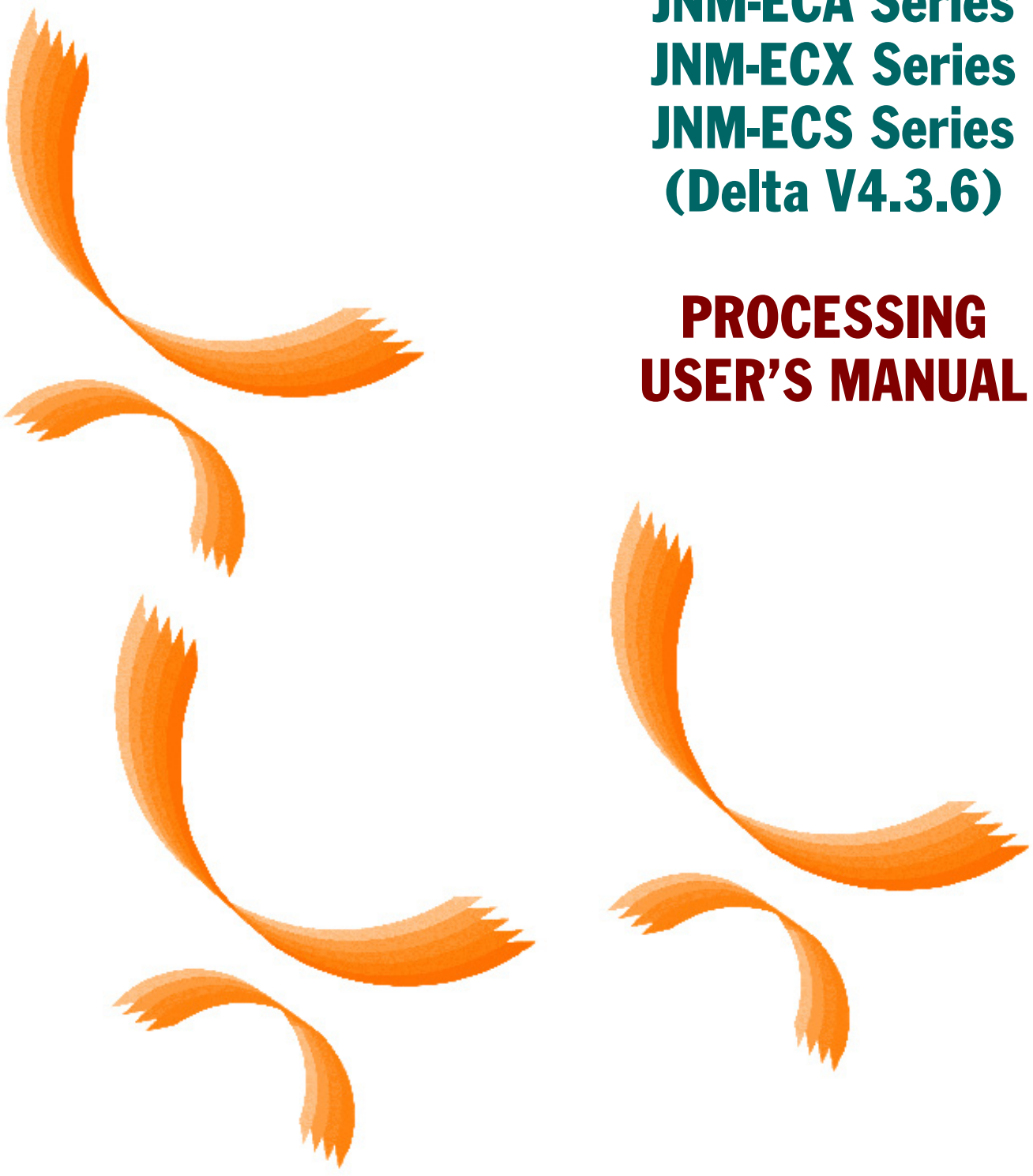
JNM-ECA Series
JNM-ECX Series
JNM-ECS Series
(Delta V4.3.6)

PROCESSING USER'S MANUAL



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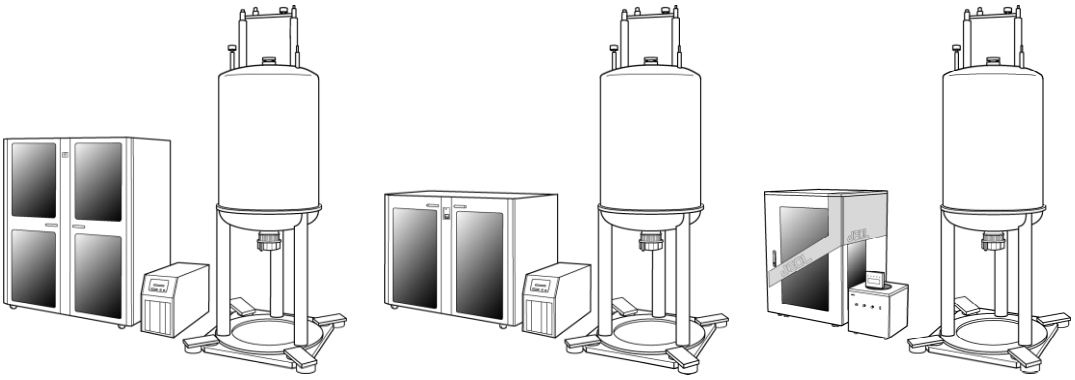

JNM-ECA Series JNM-ECX Series JNM-ECS Series

This manual is intended to help users gain a deeper understanding of the ECA/ECX/ECS-NMR system, so they can make better use of its functions for data processing.

Please be sure to read this instruction manual carefully, and fully understand its contents prior to the operation or maintenance for the proper use of the instrument.

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JEOL Ltd. 1-2, Musashino 3-chome, Akishima, Tokyo 196-8558 Japan
Telephone: 81-42-543-1111 Facsimile: 81-42-546-3353 URL: http://www.jeol.co.jp

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NOTATIONAL CONVENTIONS AND GLOSSARY

General notations

– CAUTION – : Points where great care and attention is required when operating the device to avoid damage to the device itself.

✍ : Additional points to be remembered regarding the operation.

☞ : A reference to another section, chapter or manual.

1, 2, 3 : Numbers indicate a series of operations that achieve a task.

◆ : A diamond indicates a single operation that achieve a task.

File: The names of menus, commands, or parameters displayed on the screen are denoted with **bold** letters.

File–Exit : A command to be executed from a pulldown menu is denoted by linking the menu name and the command name with a dash (–).
For example, **File–Exit** means to execute the **Exit** command by selecting it from the **File** menu.

Ctrl : Keys on the keyboard are denoted by enclosing their names in a box.

Mouse operation

Mouse pointer: An arrow-shaped mark displayed on the screen, which moves with the movement of the mouse. It is used to specify a menu item, command, parameter value, and other items. Its shape changes according to the situation.

Click: To press and release the left mouse button.

Double-click: To press and release the left mouse button twice quickly.

Drag: To hold down the left mouse button while moving the mouse.
To drag an item, you point to an item on the screen and then drag it using the mouse.

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1.1 DELTA START UP AND EXIT

This section explains how to start up and exit Delta.

☞ Refer to the “Handling of Hardware Manual” and the workstation manual starting and stopping a spectrometer and a data system.

■ Starting up the Delta program

◆ Double-click on the **Delta** icon.

The Delta program will start and the **Delta Console** window opens.

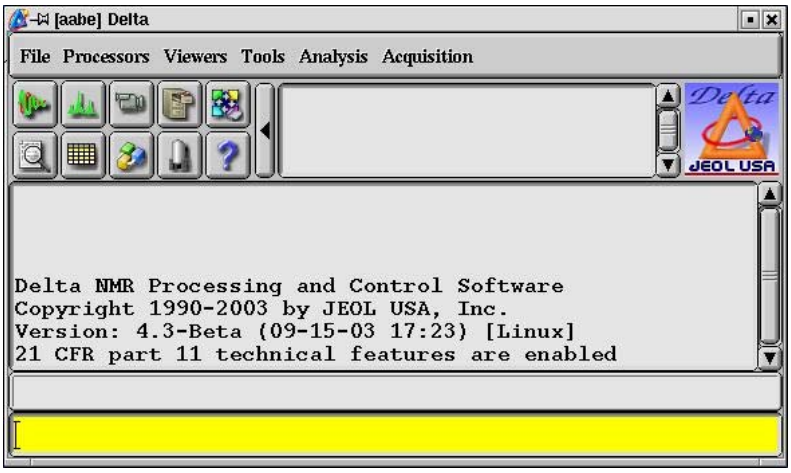
[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
Delta
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.
Version: 4.3-Beta (09-15-03 17:23) [Linux]
21 CFR part 11 technical features are enabled

Fig. 1.1 Delta Console Window

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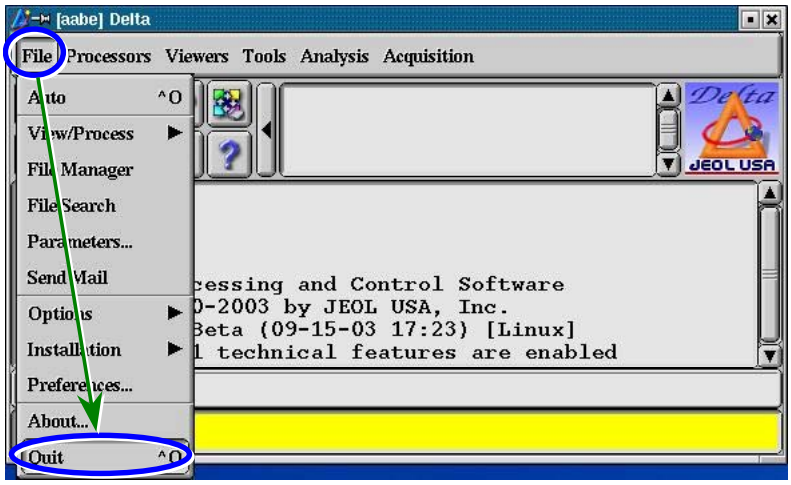
Exiting Delta

To exit Delta after measurement and processing are finished.

1. Select **File**–**Quit** in the **Delta Console** window.

Move the mouse pointer to **File** in the menu bar of the **Delta Console** window and press the left mouse button; a pull-down menu appears. Next, move the mouse pointer to **Quit** in the pull-down menu while holding down the mouse button, and release the left mouse button.



The **Confirm** window which verifies exit opens.

Fig. 1.2 Exit confirm window

2. Click on the **Ok** button.

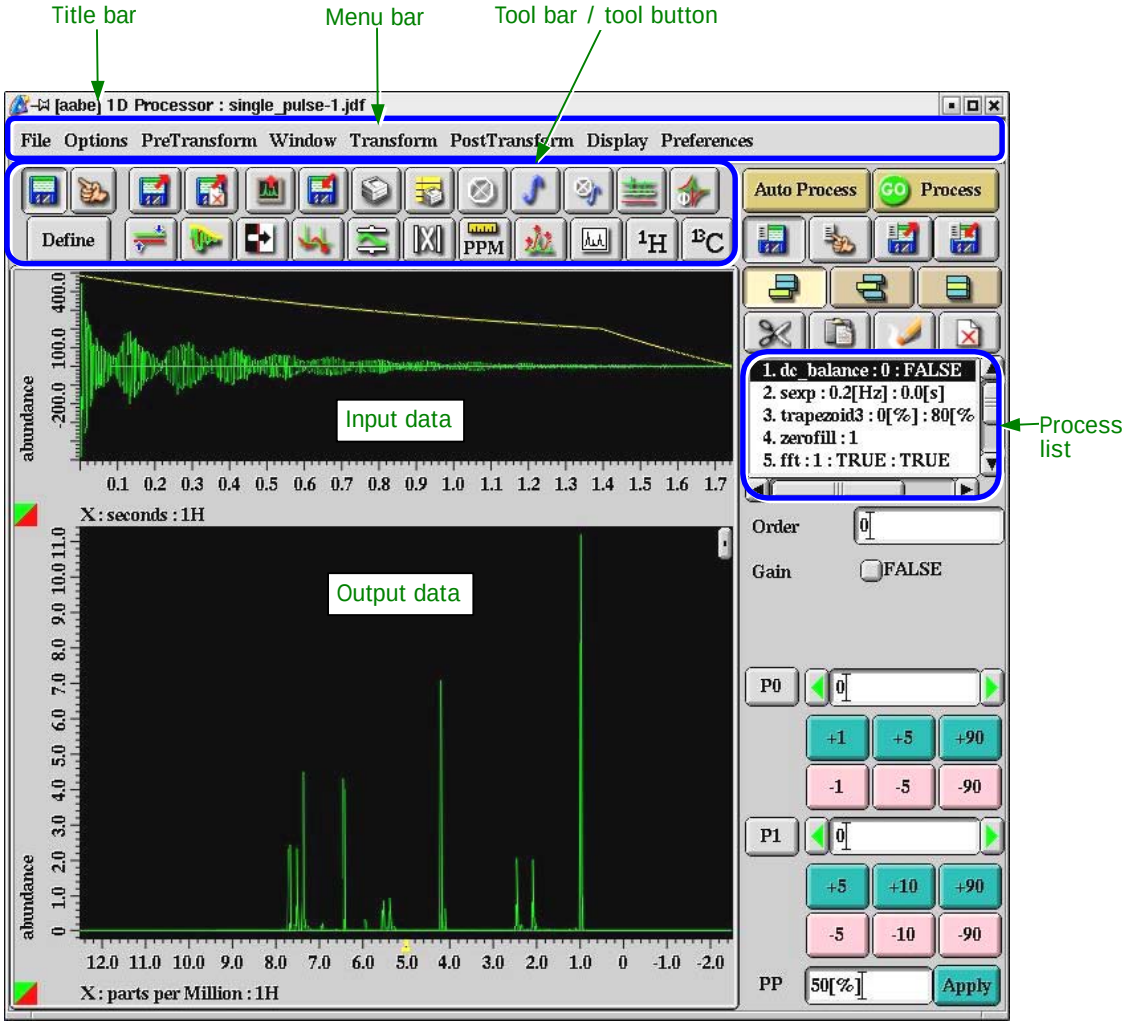
The Delta program ends.

1.2 MAIN DATA PROCESSING WINDOW

This section explains the functions of the main windows used for data processing.

1.2.1 1D Processor

When processing one-dimensional NMR data, this window is used:



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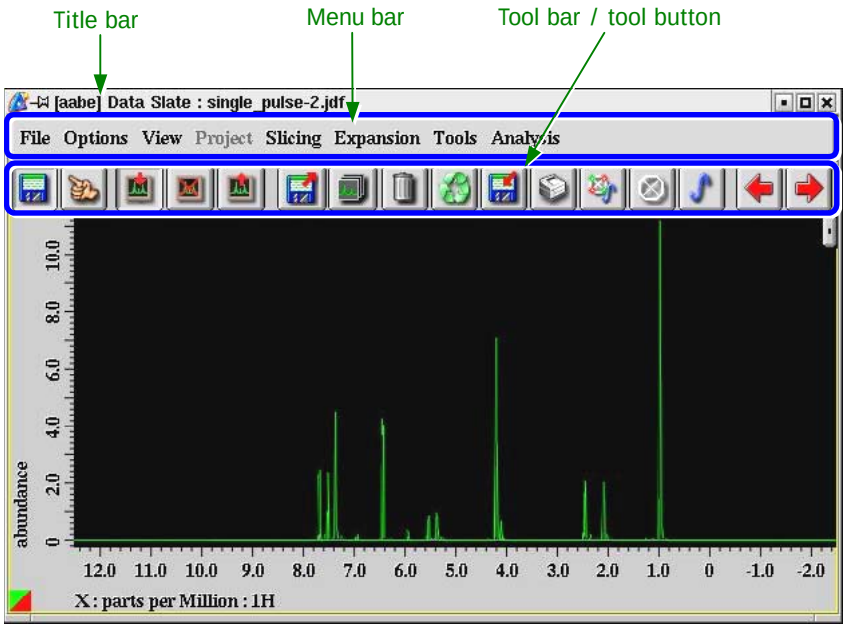
1.2.2 Data Slate

The **Data Slate** is a viewer that can be used in common irrespective of the data's dimension. In this window, two or more spectra can also be displayed.


Title bar
Menu bar
Tool bar / tool button
[aabe] Data Slate : single_pulse-2.jdf
File Options View Project Slicing Expansion Tools Analysis
abundance
0 2.0 4.0 6.0 8.0 10.0
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
X : parts per Million : 1H

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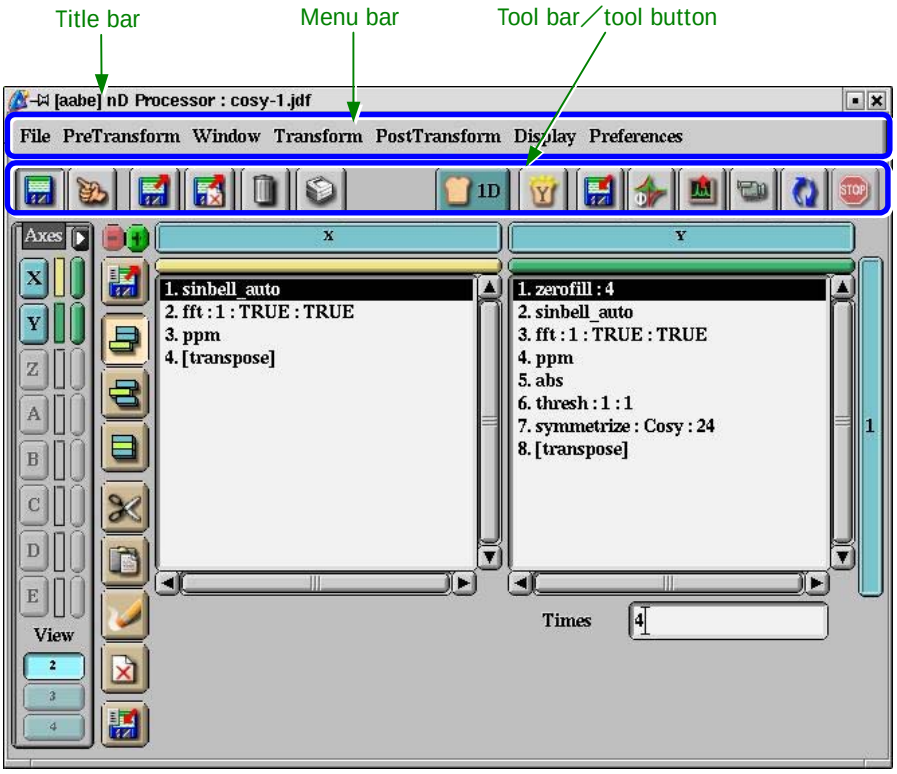
1.2.3 nD Processor

The **nD Processor** performs two to eight-dimensional data processing. Processing is performed on each axis using a process list.



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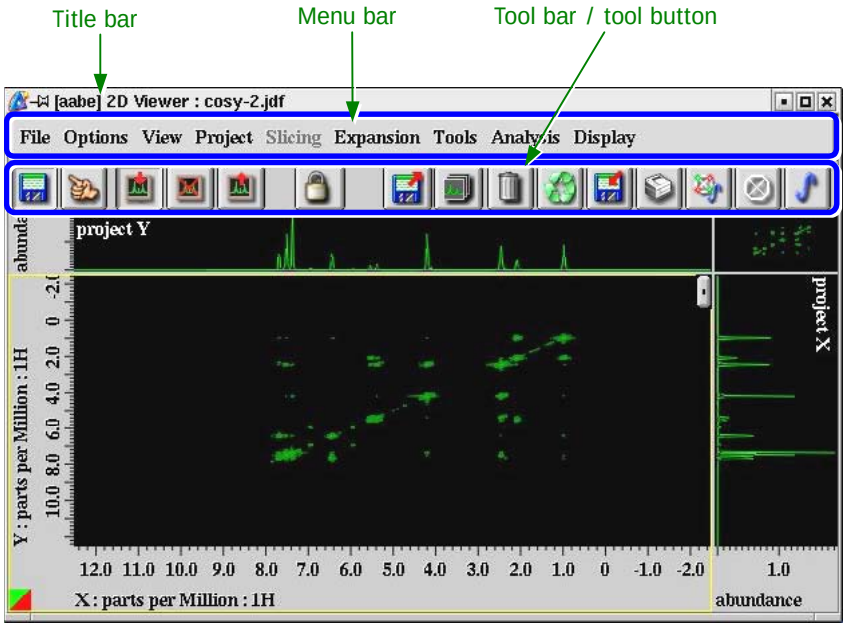
1.2.4 2D Viewer

The **2D Viewer** displays two-dimensional data. The spectra displayed are two-dimensional and one-dimensional data: slice data, projection data, or high resolution NMR.


Title bar
Menu bar
Tool bar / tool button
[aabe] 2D Viewer : cosy-2.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
project X
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

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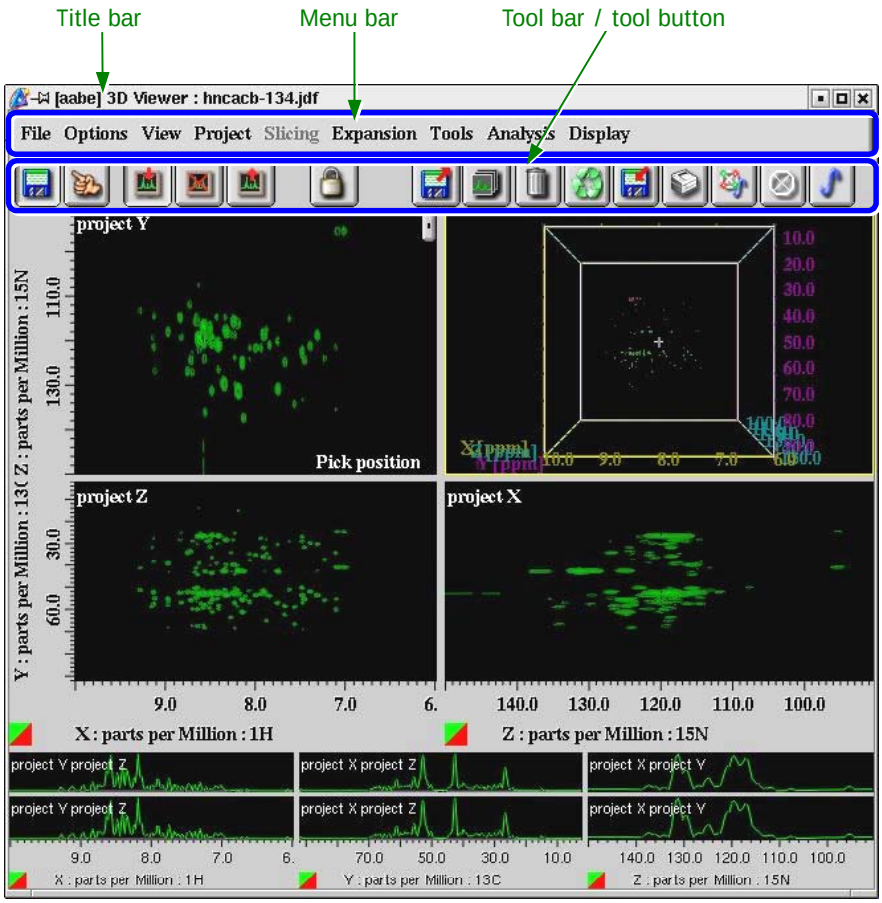
1.2.5 3D Viewer

The **3D Viewer** displays three-dimensional data. The data displayed are three-dimensional spectrum and three-dimensional projections (two-dimensional or one-dimensional projections). Moreover, slice data can also be displayed on a projection area.


Title bar
Menu bar
Tool bar / tool button
[aabe] 3D Viewer : hncacb-134.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
Pick position
project Z
project X
Y : parts per Million : 13C Z : parts per Million : 15N
X : parts per Million : 1H
Z : parts per Million : 15N
project Y project Z
project X project Z
project X project Y

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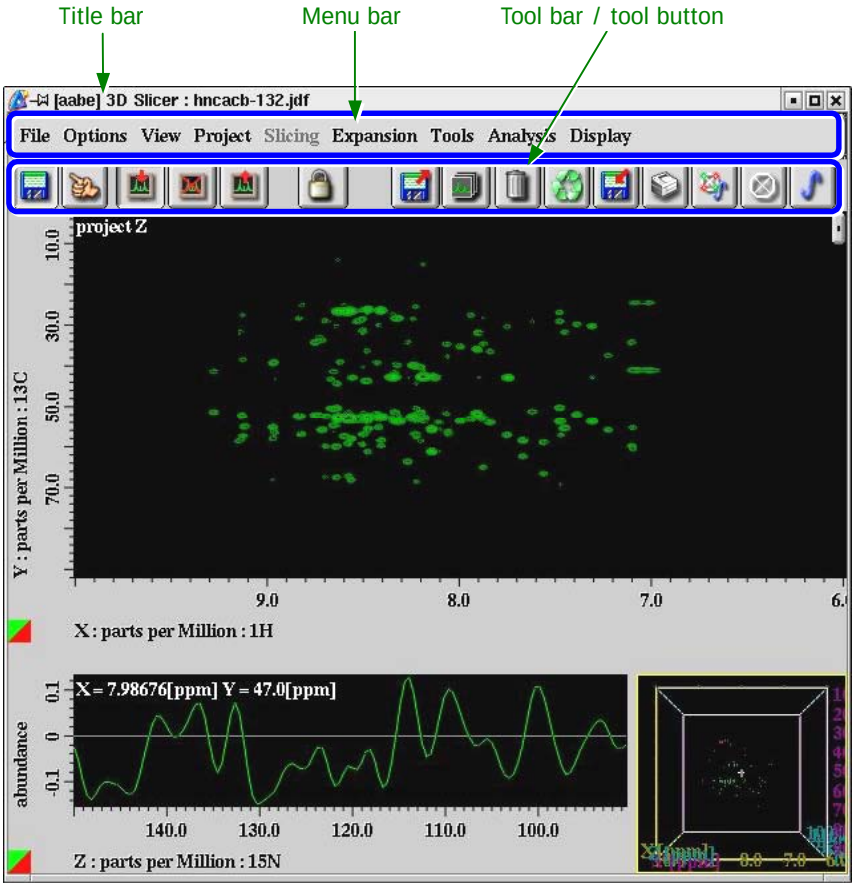
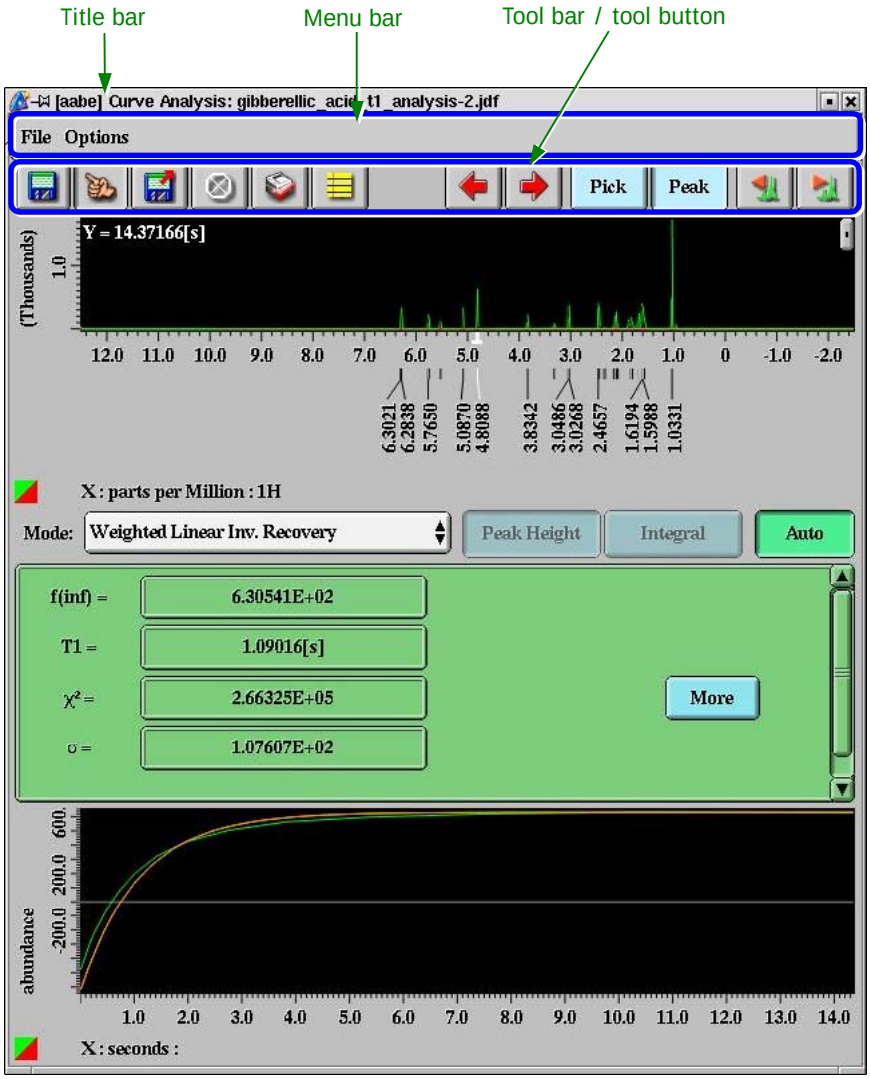
1.2.6 3D Slicer

The **3D Slicer** displays a slice of three-dimensional data. The spectra displayed are three-dimensional data and the two-dimensional or one-dimensional slice data.


Title bar
Menu bar
Tool bar / tool button
[aabe] 3D Slicer : hncacb-132.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Z
Y : parts per Million : 13C
X : parts per Million : 1H
X = 7.98676[ppm] Y = 47.0[ppm]
abundance
Z : parts per Million : 15N

1.2.7 Curve Analysis Tool

The **Curve Analysis Tool** is the tool for performing data processing of relaxation-time measurement data and diffusion data.



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1.3 CHANGING A DISPLAY

This section explains how to expand or transfer a spectrum.

1.3.1 Cursor Tool

Using a mouse pointer, the cursor tool changes the function for data processing, such as expansion, transfer, peak detection, and integration of a spectrum.

■ Cursor tool display

◆ Move the mouse pointer to the processing data display range.
The cursor tool appears on the top right in the processing data display range.

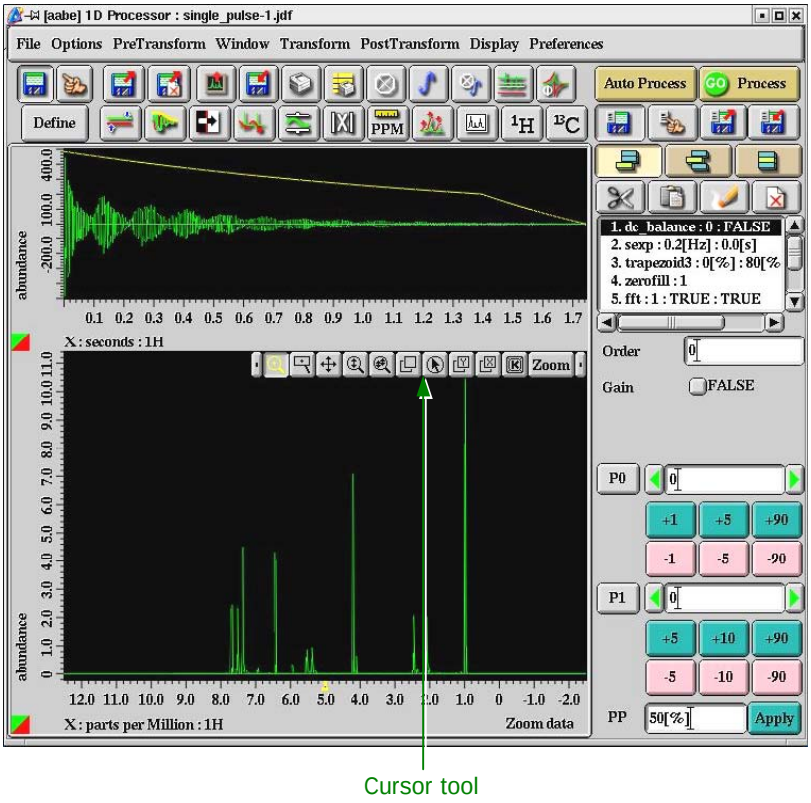

Fig. 1.3 Cursor tool in the processing data display range

The cursor tool consists of the buttons shown in the following figure:

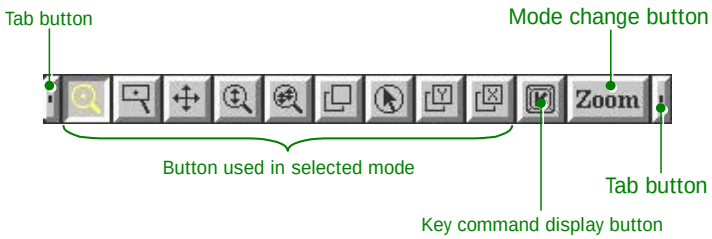

Fig. 1.4 Cursor tool

The mode change buttons accesses the function for 13 different modes.
These modes have buttons for displaying key commands.
These buttons corresponding to each mode are located to the left side of the key command display button.
There are tab buttons for minimizing the cursor tool at both ends.

Minimizing a cursor tool

The cursor tool can be minimized when it obscures the peak in a spectrum.

- Click on the tab button at the left end of the cursor tool.
  The cursor tool changes to the display only a tab button.

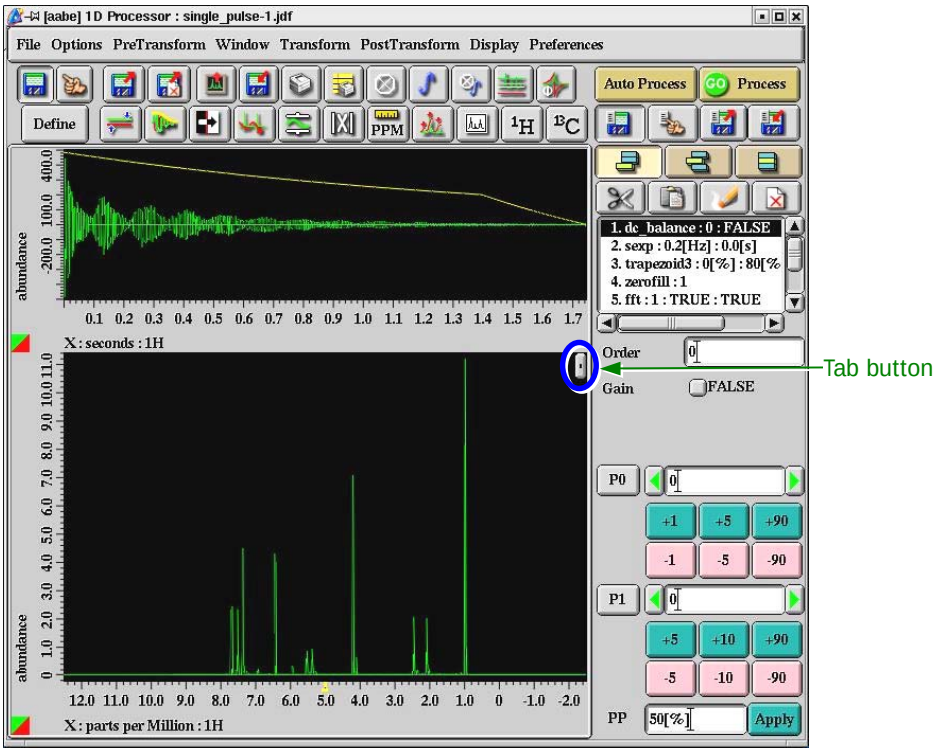

Fig. 1.5 Minimized cursor tool

Return to normal display from minimized display

- Click on the tab button with the mouse again.
  The cursor tool returns to the original display.

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1.3.2 Changing Modes and Selecting Mode Buttons

■ Changing modes in the cursor tool

1. Move the mouse pointer to the mode change button at the right end of the cursor tool; press and hold down the left mouse button.

The following 13 modes are displayed the pull-down menu:

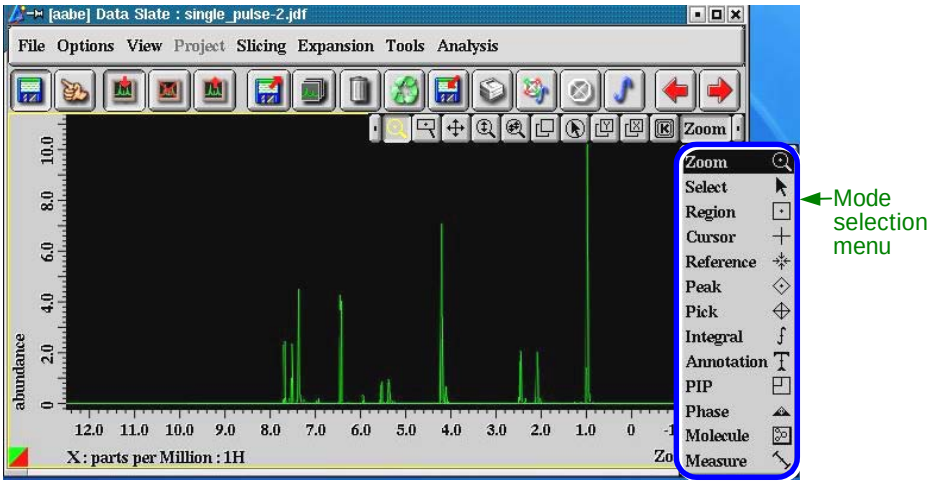


Fig. 1.6 Mode selection menu

Mode	Explanation
Zoom	Expansion, reduction or transfer of a spectrum.
Select	Data and geometry selection.
Region	For displaying the selected range to another geometry.
Cursor	For baseline correction and displaying the difference between two points.
Reference	Setting operation for the chemical shift reference of the axis marker.
Peak	For peak picking.
Pick	For slice of 2D data and reading peak position.
Integral	For integration.
Annotation	For display of an explaining sentence on the geometry.
PIP	For display of the geometry's selected range.
Phase	For phase correction.
Molecule	For display of geometry's structural or molecular formula.
Measure	For measuring data.

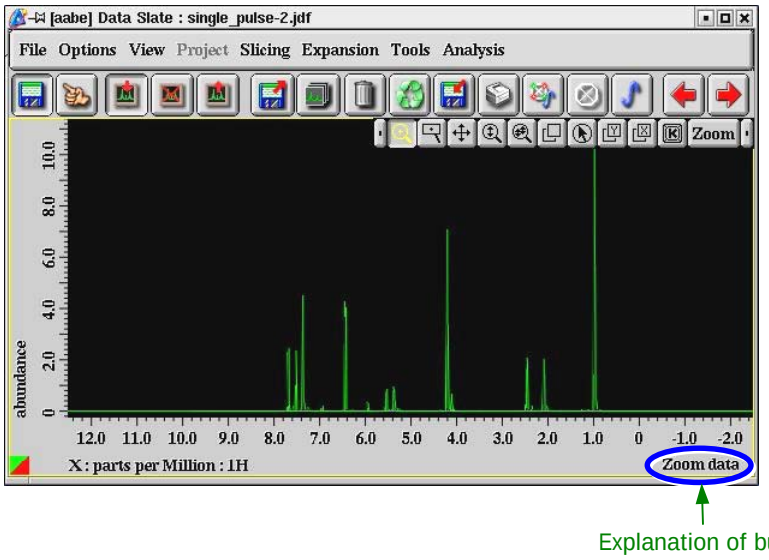
2. Move the mouse pointer to the mode you want to select while holding it down, then release the mouse button.

The display of a cursor tool changes to the selected button in the mode.

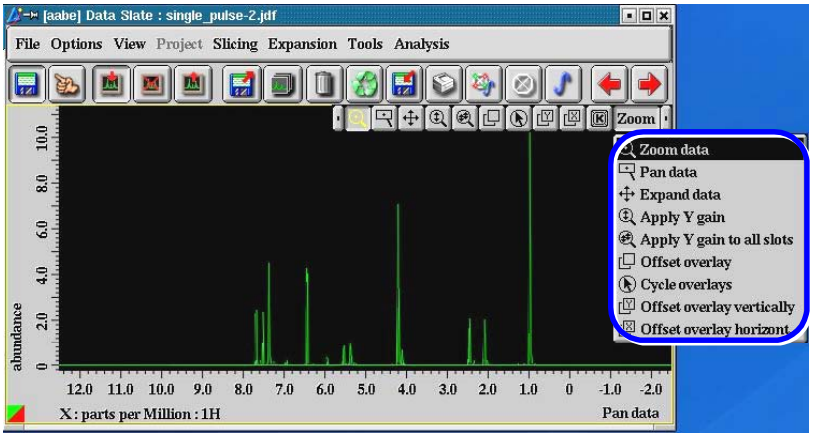
Selecting a button to use

- Click on a button you want to use.

  This changes the selection display. A tag explaining the selected button is displayed on the bottom right of the data processing display range.



If you press the mode change button with the central mouse button, a list offering a brief explanation of the button used in the mode currently selected will be displayed. The button you want to use can also be selected from the display.



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1.3.3 Key Command Display Button

The key command changes the functions.

■ Executing the key command

1. Move the mouse pointer to the button.
2. Press and hold down the left mouse button.
   The key command appears.
3. Move the mouse pointer to the target key command while holding it down, and release the mouse button.
   The selected key command is executed.

✍ This operation is the same as pressing the key displayed by [ ] in each key command on the keyboard.

■ How to use a typical key command

- **To return a spectrum to the initial state display using the Reset View [Home] key command**

  1. Move the mouse pointer to the button.
  2. Press and hold down the left mouse button.
     The key command appears.
  3. Move the mouse pointer to the **Reset View [Home]**, and release the mouse button.
     The spectrum returns to the initial state display.

  ✍ This operation is the same as pressing the Home key on the keyboard.

- **To Return a spectrum to the display in the preceding state using the Unzoom [Bksp] key command**

  1. Move the mouse pointer to the button.
  2. Press and hold down the left mouse button.
     The key command appears.
  3. Move the mouse pointer to **Unzoom [Bksp]**, and release the mouse button.
     The spectrum returns to the display in the preceding state.

  ✍ This operation is the same as pressing the BackSpace key on the keyboard.

- **To Optimize the maximum peak displayed using the Scale Y [End] key command**

  1. Move the mouse pointer to the button.
  2. Press and hold down the left mouse button.
     The key command appears.
  3. Move the mouse pointer to the **Scale Y [End]**, and release the mouse button.
     The maximum peak of the spectrum range currently displayed is expanded or reduced in the vertical direction so that it may fit in the processing data display range.

  ✍ This operation is the same as that performed by pressing the End key on the keyboard.

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1.3.4 Mode Buttons

This section explains the function of each mode in button of the cursor tool.

■ Zoom mode

This mode performs an expansion, reduction, and transfer of a spectrum.

Button	Button name	Explanation
	Zoom data	Performs expansion of the spectrum in the vertical, horizontal ,or both direction.
	Pan data	Performs transfer of spectrum in the vertical or horizontal direction.
	Expand data	Performs expansion and reduction of the spectrum in the vertical or horizontal direction.
	Apply Y gain	Performs expansion and reduction of a spectrum in the vertical direction.
	Apply Y gain to all slots	Performs expansion and reduction of all spectra that have overlapped in the vertical direction in the **Data Slate** window.
	Offset overlay	Changes the display positions of the spectrum selected from the spectra that overlap in the **Data Slate** window in the vertical and horizontal direction.
	Cycle overlays	Selects the target spectrum when overwriting the spectra in the geometry.
	Offset overlay vertically	Changes the display position of the spectrum selected from spectra in the **Data Slate** window that overlap in the vertical direction.
	Offset overlay horizontally	Changes the display position of the spectrum selected from spectra in the **Data Slate** window that overlap in the horizontal direction.

■ Select mode

This mode selects a data and a geometry.

Button	Button name	Explanation
	Select a geometry	Selects the target geometry.
	Cycle Overlays	Selects the target spectrum of operation when overwriting in the one geometry.
	Apply box analysis	Specifies the target when limiting the range in one geometry. For example, the target range of the **Zero Region** function in the **2D viewer** window may be specified.

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Region mode

This mode displays the selected range to another geometry:

Button	Button name	Explanation
	Create a region	Specifies the range when creating a PIP box. In the **Presentation Manager** window, the range is specified in the creation of a **Box** or **2D Phaser**.
	Move/Resize a region	Performs transfer of the **PIP** box, and changes its size. In the **Presentation Manager** window, transfer of the **Box** and size change are performed.
	Delete a region	Deletes the PIP box. The **Box** is deleted in the **Presentation Manager** window.

Cursor mode

This mode performs the operation for baseline correction, and display of the difference between two points:

Button	Button name	explanation
	Create a cursor	Creates a new cross cursor.
	Move a cursor	Moves the position of the cross cursor.
	Select a cursor	Selects the cross cursor.
	Delete a cursor	Deletes the cross cursor.

Reference mode

This mode sets up the reference of the chemical shift for a axis marker.

Button	Button name	Explanation
	Grab a position for reference	Reads the frequency of the position specified in a spectrum as a reference.
	Paste a reference	Pastes the reference on the specified position.
	Paste a reference to nearest peak	Pastes the reference on the peak in the nearest peak of the specified position.
	Paste a reference to all geometries	Pastes the reference on all the geometry's overlapped display.
	Cycle overlays	If you click on the geometry's overlapped display, the selected geometry will move to the next.

Peak mode

This mode performs the peak picking operation.

Button	Button name	Explanation
	Create a peak	Sets up the top of the peak in the neighborhood as a new peak.
	Force create a peak	Adds the specified position as a peak.
	Delete a peak	Deletes a peak.
	Adjust the peak threshold	Adjusts the peak level to detect in the statistics set up at peak picking.
	Adjust the noise threshold	Adjusts the noise level in the statistics set up at peak picking.
	Adjust the baseline/thresholds	Adjusts the base level in the statistics set up at peak picking
	Select peaks	Selects setting peak.
	Select more peaks	Selects more peaks in the state in which the peak is selected.
	Unselect peaks	Cancels selection.

Pick mode

This mode performs the slice operation of two-dimensional data and reading of a peak position.

Button	Button name	Explanation
	Pick position	Reads peak position.
	Copy position to buffer	Copies the read peak position.
	Copy position of nearest peak to buffer	Copies the nearest peak position from the specified peak position.
	Set datadex slice point	Sets the datadex to slice point.
	Spear datadexed file	Displays a peak position in the datadex.
	Copy relative to center of ruler	Reads the distance of the selected peak from the center of a spectrum, and pastes on the cut-and-paste buffer of the **Delta Console** window.
	Pick lower Contour Bound	Sets up the lowest position of a contour line level from a projection or slice data.
	Pick Upper Contour Bound	Sets up the highest position of a contour line level from a projection or slice data.
	Pick Selected Contour Threshold	Sets up the contour line level position selected in the **Level Tool** window from a projection or slice data

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Integral mode

This mode performs the integration operation.

Button	Button name	Explanation
	Create an integral	Sets up a new integration range.
	Delete an integral	Delete specified an integration range.
	Change the slope of an integral	Sets up the baseline slope of an integration range. Corrects the slope changing the base point marker.
	Adjusting an integral	Adjusts an integration range.
	Split integral two	Cuts the selected integration curve in an arbitrary position.
	Gain integrals in Y	Sets up the size of the vertical direction in the integration range.
	Change offset of the integrals	Sets up the position of the integration curve on an integrals spectrum.
	Adjust the peak threshold	Adjusts the peak level to detect in the statistics set up at peak picking.
	Adjust the noise threshold	Adjusts the noise level to detect in the statistics set up at peak picking.
	Adjust the baseline / thresholds	Adjusts the baseline level to detect in the statistics set up at peak picking.
	Select integrals	Select the integration range set up.
	Select more integrals	Selects more integrals in a selected integration range.
	Unselect integrals	Cancels the selected integration range.

Annotation mode

This mode performs the operation that displays explanation note on the geometry.

Button	Button name	Explanation
	Create a text annotation	Enters a text in any where in the data processing display range.
	Edit a text annotation	Changes a text.
	Create a Rectangle	Creates a rectangle in an arbitrary places of the data processing display range.
	Create a Line	Creates s straight line in an arbitrary places of the data-processing display range.
	Create an Arrow	Creates an arrow in the arbitrary place of the data processing display range.
	Create Double Arrow	Creates a two-sided arrow in an arbitrary place of the data processing display range.

Button	Button name	Explanation
	Move/Resize Annotation	Moves the text, or changes its size.
	Delete annotation	Deletes a text.
	Select annotation	Selects the text.
	Add Select annotation	Selects a text in the state in which text is selected.
	Deselect annotation	Cancels selection

■ PIP mode

This mode displays the selected range to the same geometry.

Button	Button name	Explanation
	Create a PIP by zoom region	Creates the partial spectrum (PIP box) from the whole spectrum region.
	Move/Resize PIP zoom region	Moves the PIP box made in the **Create PIP by zoom region,** or changes its size.
	Create a PIP	Inserts an entire spectrum in the arbitrary positions of the data display range. The inserted spectrum can change a range in **Zoom** mode.
	Move/Resize the PIP	Moves the PIP box made in **Create PIP,** or changes its size.
	Delete the PIP	Deletes the PIP box.

■ Phase mode

This mode corrects a phase.

Button	Button name	Explanation
	Adjust the Phase PP value	Adjusts display phase parameter PP.
	Adjust the Phase P0 value	Corrects 0 order phase (P0) parameter.
	Adjust the Phase P1 value	Corrects first order (P1) parameter.
	Pick position	Reads a peak position.

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Molecule mode

This mode displays a structural formula and a molecular formula to the geometry.

Button	Button name	Explanation
	Create a Molecule window	Specifies the range when creating the **Molecule** window.
	Move/Resize the Molecule window	Moves the **Molecule** window, and changes its size.
	Select the Molecule window	Selects the **Molecule** window.
	Delete the Molecule window	Deletes the **Molecule** window.
	Select an Atom	Selects atom in the **Molecule** window.
	Select more peaks	Selects a peak.
	Unselect peaks	Cancels peak selection.

Measure mode

This mode creates a measure (ruler) on the data.

Button	Button name	Explanation
	Create a Measure	Creates the measure range in the arbitrary places of the data-processing display range.
	Create a Measure in X	Creates a measure range in the X direction.
	Create a Measure in Y	Creates a measure range in the Y direction.
	Resize a Measure	Changes a measure range.
	Resize a Measure in X	Changes a measure range in the X direction
	Resize a Measure in Y	Changes a measure range in the Y direction
	Rotate a Measure	Changes the measure direction.
	Select a Measure Near the Cursor	Selects a measure set.
	Unselect a Measure	Cancels the measure range.
	Delete a Measure	Deletes the measure range.

1.3.5 How to Use the Cursor Tool

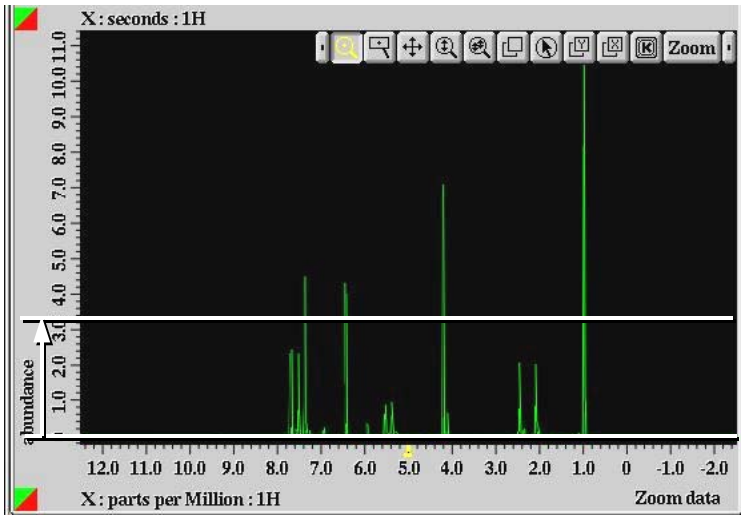
1.3.5a Expanding a spectrum

This section explains the expansion method using the **Zoom data** mode of the cursor tool.

Shortcut to the **Zoom data** button
Pressing the Shift key in the keyboard changes the mode to **Zoom data**.

■ Vertical expansion of a spectrum

1. Click on the button with the left mouse button.
2. Move the mouse pointer to the expansion start position on the Y ruler.
3. Press and hold down the left mouse button.
   The horizontal cursor appears.
4. Move the mouse pointer to an expansion end position, and release the mouse button.



The cursor range is expanded in the vertical direction.

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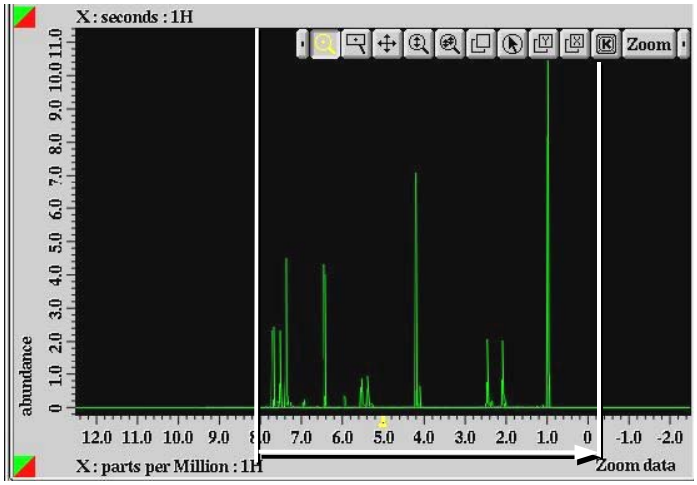
Horizontal expansion of a spectrum

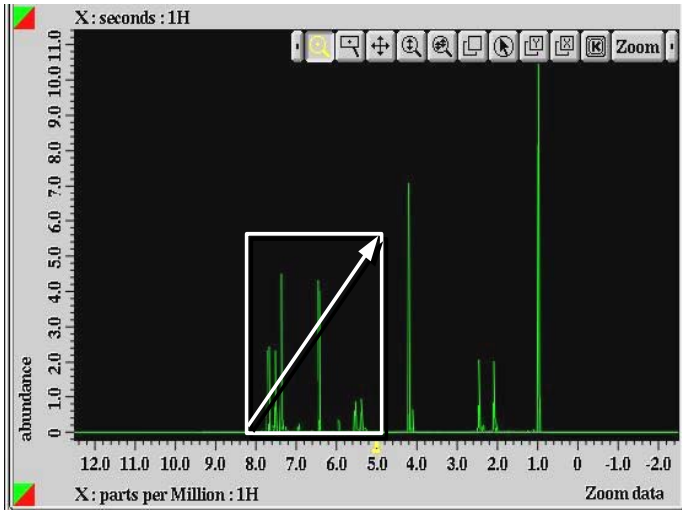
1. Click on the button with the left mouse button.
2. Move the mouse pointer to the expansion start position on the X ruler.
3. Press and hold down the left mouse button.
   The vertical cursor appears.
4. Move the mouse pointer to an expansion end position, and release the mouse button.



The cursor range will be expanded in the horizontal direction.

Expansion of a spectrum in the both vertical and horizontal direction

1. Click on the button with the left mouse button.
2. Move the mouse pointer to the expansion start position in the processing data display range.
3. Press and hold down the left mouse button.
   The rectangular cursor appears.
4. Move the mouse pointer to an expansion end position as it is, and release the mouse button.



The cursor range will be expanded in both the vertical and horizontal directions.

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1.3.5b Moving a spectrum

How to move a spectrum is explained using the **Pan data** mode.

■ Moving a spectrum in the vertical direction.

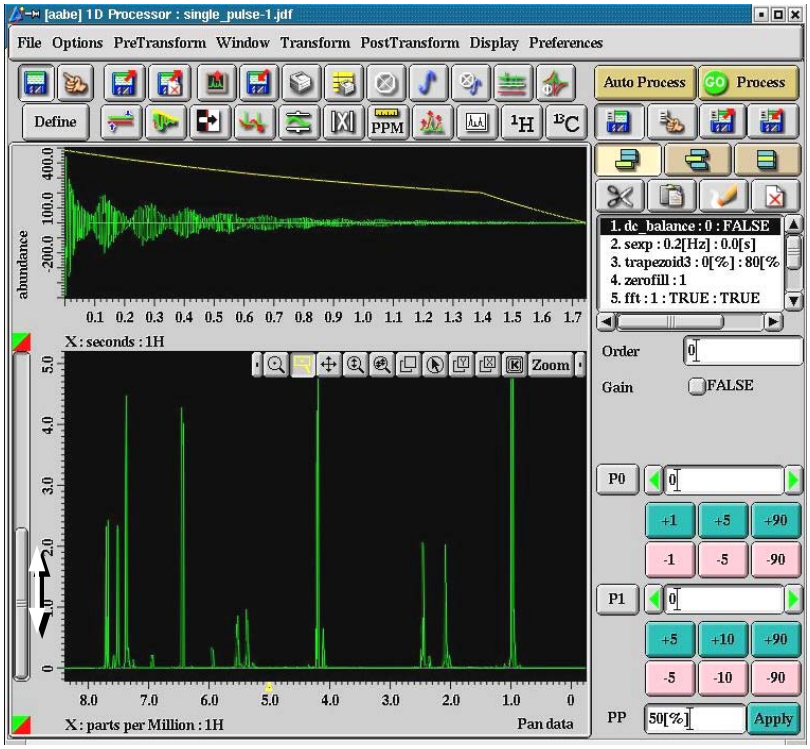
1. Click on the button using the left mouse button.

2. Move the mouse pointer onto the Y ruler.
It does not operate in the processing data display range.

3. Press and hold down the left mouse button.
The expansion ruler appears.

4. Move the mouse pointer up and down while holding down the mouse button.
Synchronized with moving an expansion ruler, a spectrum may be moved up and down.

When the spectrum is not expanded in the vertical direction, the expansion ruler does not move.



5. Release the mouse button.
The movement ends.

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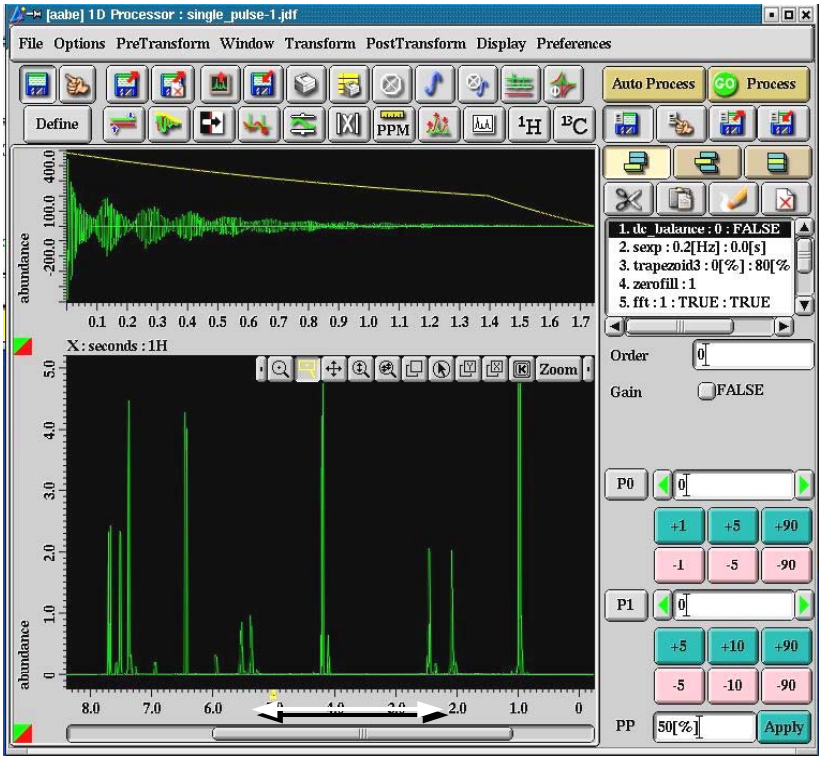
Moving a spectrum in the horizontal direction

1. Click on the button using the left mouse button.
2. Move the mouse pointer onto the X ruler.
   It does not operate in the processing data display range.
3. Press and hold down the left mouse button.
   The expansion ruler appears.
4. Move the mouse pointer right and left while holding down the mouse button.
   Synchronized with moving an expansion ruler, a spectrum may be moved right and left.
   When the spectrum is not expanded in the horizontal direction, the expansion ruler does not move.



5. Release the mouse button.
   Movement of expansion ruler ends.

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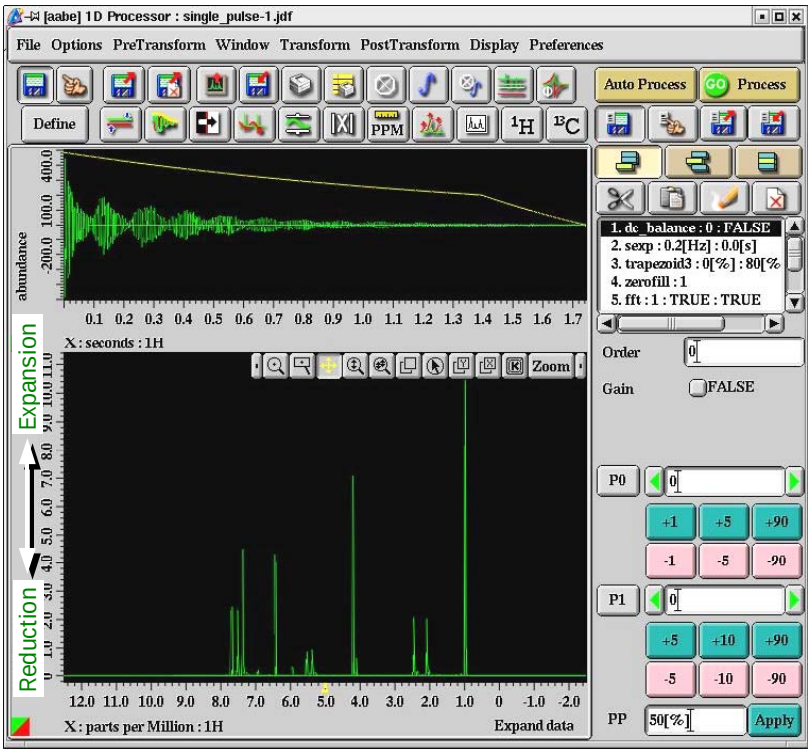
1.3.5c Expansion and reduction of a spectrum

This section explains how to expand and reduce a spectrum using the **Expand data** mode.

■ Vertical expansion and reduction of a spectrum

1. Click on the button with the left mouse button.
2. Move the mouse pointer onto the Y ruler.
3. Press and hold down the left mouse button and move the mouse pointer up and down.

   Synchronized with moving the mouse pointer, a spectrum may be expanded and reduced in the vertical direction.



4. Release the mouse button.

   Expansion and reduction end.

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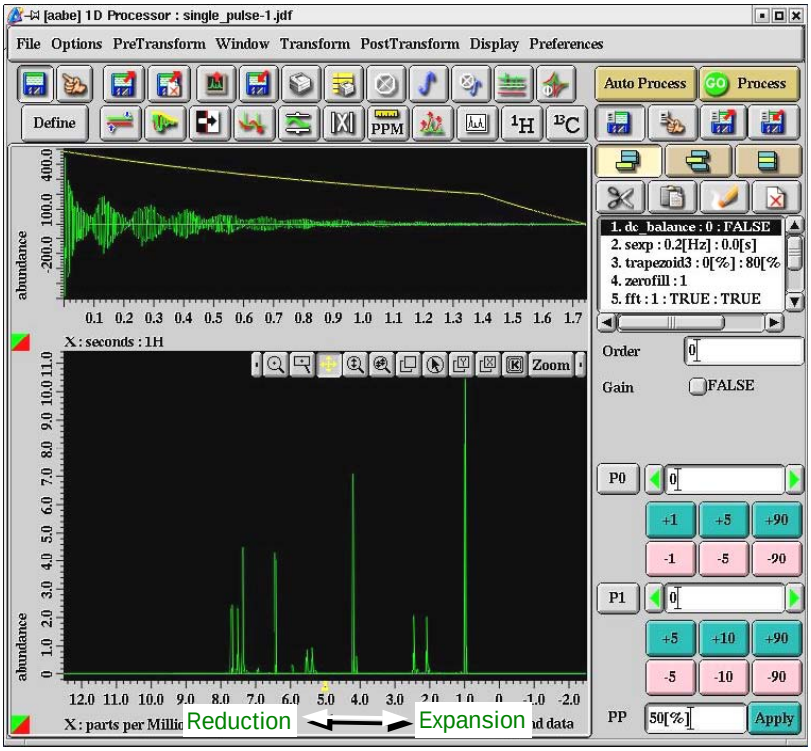
Horizontal expansion and reduction of a spectrum

1. Click on the button with the left mouse button.
2. Move the mouse pointer onto the X ruler.
3. Press and hold down the left mouse button and move the mouse pointer to the right and left.

   Synchronized with moving the mouse pointer, a spectrum may be expanded and reduced in the horizontal direction.



4. Release the mouse button.

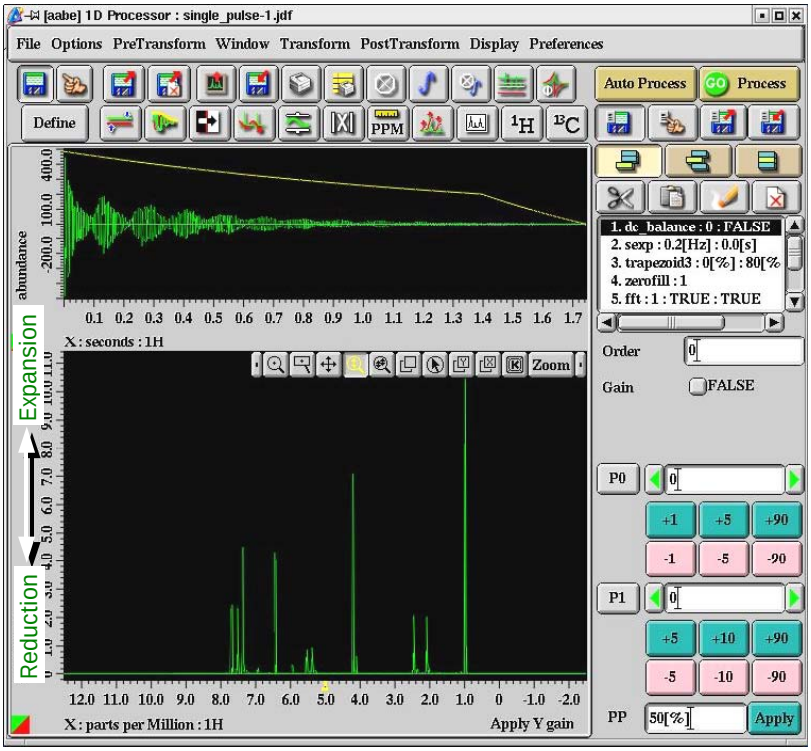
   Expansion and reduction ends.

1.3.5d Changing the Y gain

This section explains how to change the Y gain of a spectrum using the **Apply Y gain** mode.

■ Vertical expansion and reduction of a spectrum

1. Click on the button with the left mouse button.
2. Move the mouse pointer onto the Y ruler.
3. Press and hold down the left mouse button.
4. Move the mouse pointer up and down.
   The Y gain of a spectrum changes.



5. Release the mouse button.
   Change of the Y gain of a spectrum ends.

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1.4 THE PROCESS LIST

This section explains the process list used as fundamentals for data processing in Delta.

1.4.1 Process List

The process list describes various kinds of processing contents and the conditions for data processing in Delta. Processing contents and conditions are described in the order of processing.

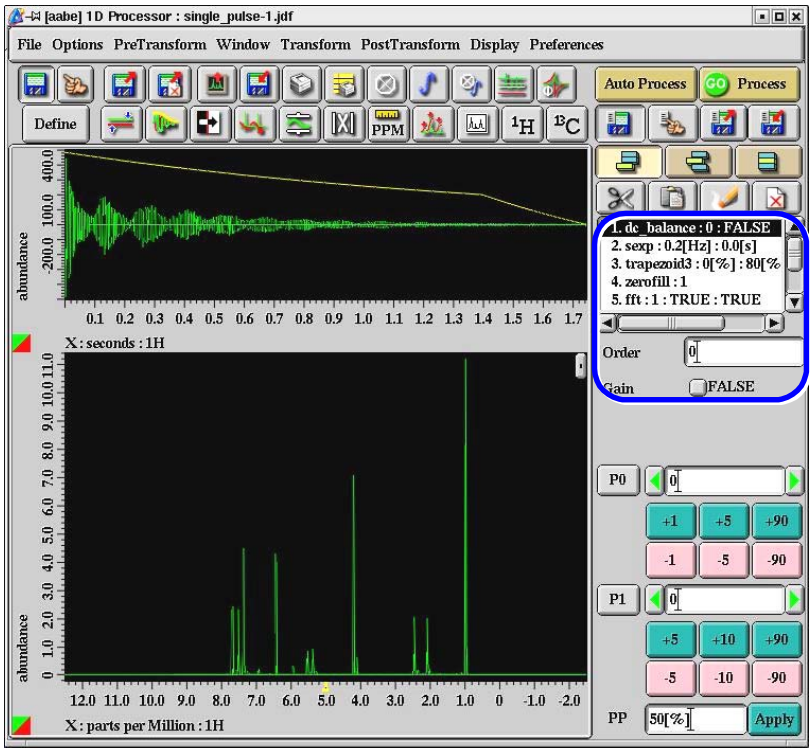

Fig. 1.7 Process list in a 1D Processor

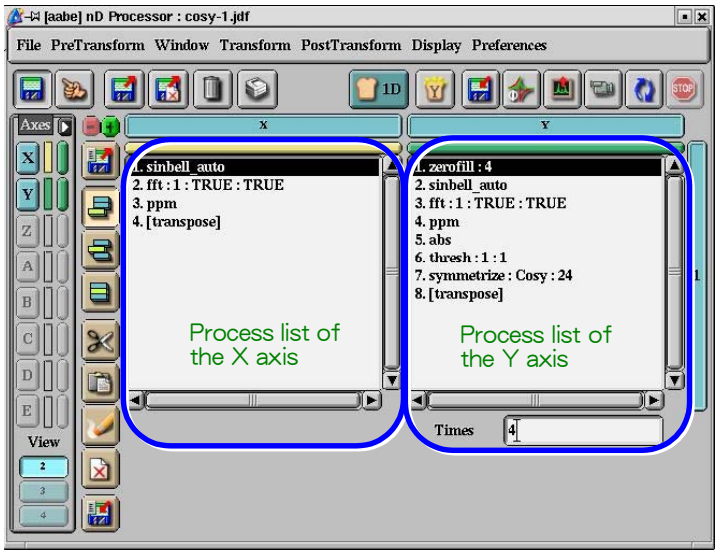

Fig. 1.8 Process list in nD Processor

The process list, in which contents of standard data processing are described for typical measurement data, is supplied. This process list is called the “standard process list”.
The standard process list is saved in the Global Process List directory.
Moreover, the standard process list suiting the measurement is set to a typical measurement sequence. When measurement was complete, data will upload to a workstation, standard processing set up will be performed automatically.
Seeing the processing data displayed, processing conditions can be made optimal for data measurement, or another new data processing task can be added.
Thus, fundamental data processing for Delta will perform the process list set up. Moreover, changing the data processing conditions described in the process list will perform a change of the processing conditions.
The processing contents can be changed, or the newly created process list can also be saved to a file as another process list. When performing data processing with the same conditions, processing becomes possible by an easy operation which reads the purposed process list.

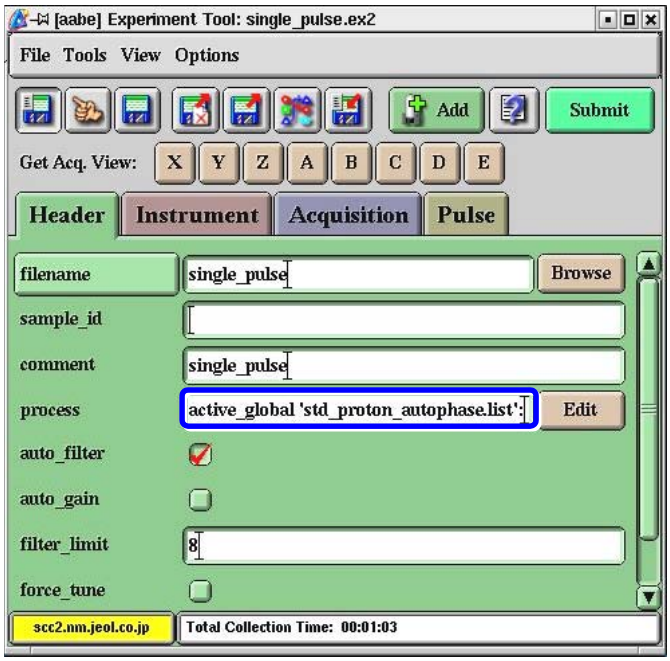

Fig. 1.9 Process list set in the sequence

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1.4.2 Process List Composition

1.4.2a Process list

A process list in **1D Processor** describes the contents for data processing in the input window. The results of processing are displayed on an output window.

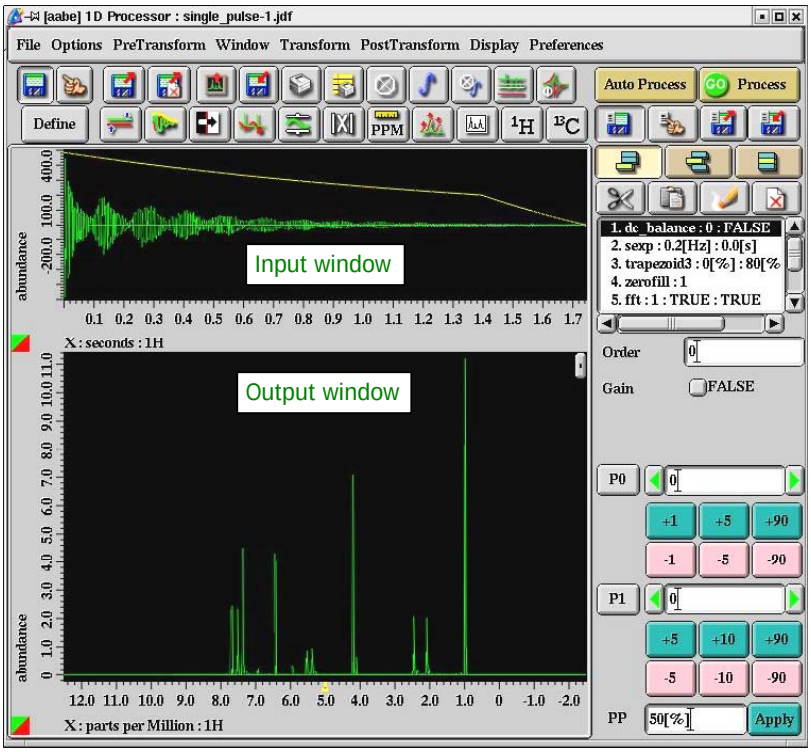
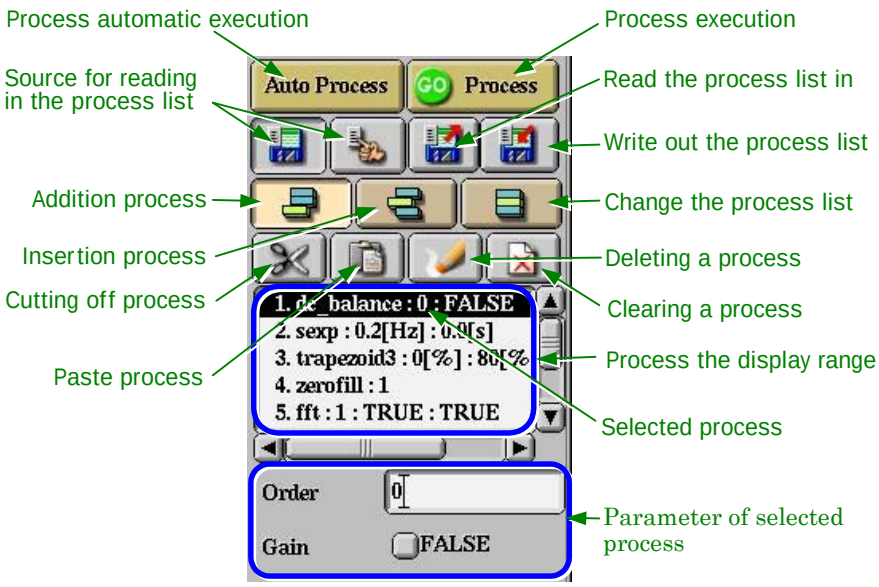


Fig. 1.10 1D Processor window

In the example above, the result for data processing, such as FFT and phase correction, described in the process list and performed on a FID in the input window, is displayed on the output window.



1.4.2b Process control button

This section explains the process control buttons in the process list of **1D Processor**.

✍ Although the process control button of **nD Processor** is fundamentally the same as that of **1D Processor**, there is a slight difference. Refer to the later section "■In the **nD Processor** window".

Button	Button name	Explanation
	Auto Process	The process described in the process list is applied automatically. When addition or deletion of a process is performed, re-execution of the process list is performed automatically. If a complicated process list is used, the CPU is occupied and processing may take time.
	Process	The contents of a process list are applied to input data, and display the result on an output window. When the contents of the process are changed, click on the button again, and apply the process list.
	Append	When adding a process from the pull down menu, the process is added the bottom of the process list.
	Insert	When adding the process from the pull down menu, the process is added before the selected(highlighted) process.
	Change	When adding a process from the pull down menu, the selected (highlighted) process is deleted, and the process selected replaces it.
	Cut	The selected (highlighted) process is deleted, and the deleted process is saved to the cut buffer.
	Paste	The process saved to the cut buffer is inserted before the selected (highlighted) process.
	Delete	The selected (highlighted) process is deleted. The deleted process is not saved to the cut buffer.
	Clear	All processes in the process list are deleted.

✍ The Cut button and the Paste buttons can be used only in the same process list window.

✍ The **display/phase** process in the process list of the **1D Processor** windows is displayed last on the process list, and cannot be deleted.

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1.4.3 Creating and Editing a Process List

This section explains a method for creating and editing a process list.

1.4.3a Adding the process

This section explains how to add a new process at the end of the process list.

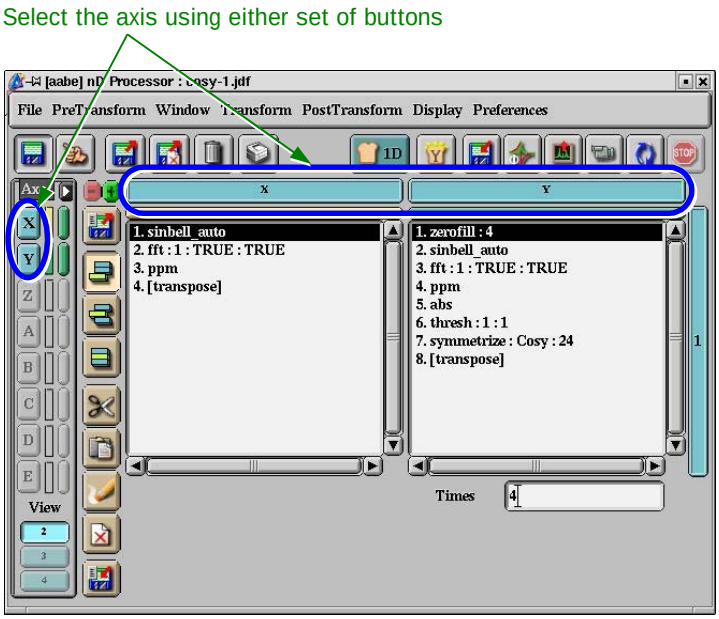
■ In the 1D Processor window

1. Click on the **Append** button in the **1D Processor** window to enter **Append** mode.
2. Select the process to add from the data processing button or menu bar.
   The selected process is added before **display/phase**.

■ In the nD Processor window

This method is explained using an example of the process list addition in two-dimensional NMR data .

1. Click on the **Append** button in the **nD Processor** window to enter **Append** mode.
2. Click on the **X** or **Y** button to select the axis to add to the process.
   X: When adding a process to the X-axis (direct observation axis).
   Y: When adding a process to the Y-axis (indirect observation axis).



3. Choose the process to add from the data-processing button or the menu bar.
   The selected processing is added before **transpose**.

1.4.3b Inserting a process

This section explains how to insert a process at the place specified in the process list.

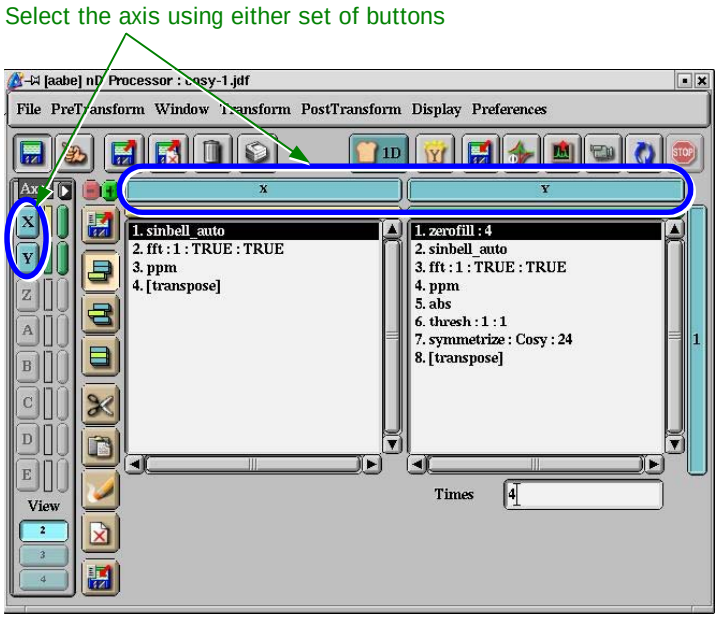
■ In the 1D Processor window

1. Click on the **Insert** button in the **1D Processor** window to enter **Insert** mode.
2. Select the process to be performed after the process to insert from the process list.
3. Select the process to insert from the data-processing button or the menu bar.
   The process selected here is inserted before the process selected in step 2.

■ In nD Processor window

This method is explained using an example of process list insertion in two-dimensional NMR data.

1. Click on the **Insert** button in the **nD Processor** window to enter **Insert** mode.
2. Click on the **X** or **Y** button to select the axis to which you want to add a process.
   X: When adding a process to the X-axis (direct observation axis).
   Y: When adding a process to the Y-axis (indirect observation axis).



3. Select the process performed after the process to insert from the process list.
4. Select the process to insert from the data-processing button or the menu bar.
   The process selected here is inserted before the process selected in step 3.

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1.4.3c Replacing the process

This section explains how to replace a process specified in the process list.

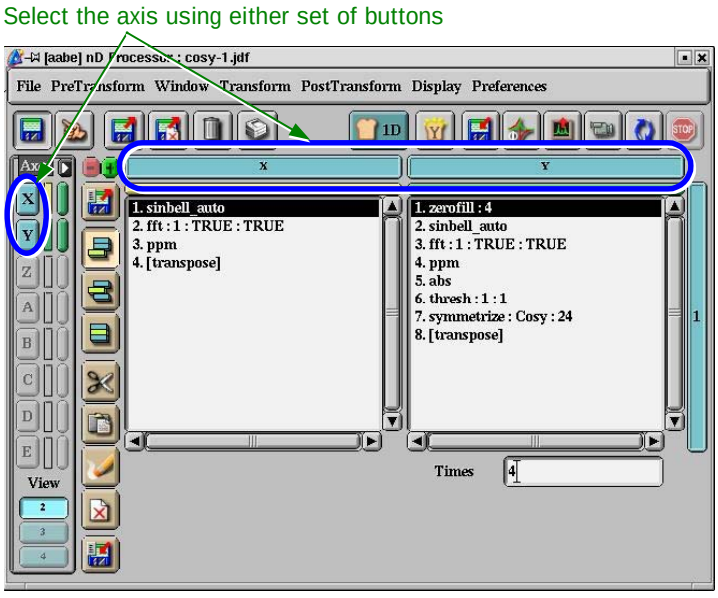
■ In the 1D Processor window

1. Click on the **Change** button in the **1D Processor** window to enter **Change** mode.
2. Select the process to replace in the process list.
3. Select the process to replace from the data-processing button or the menu bar.
   The process selected here is replaced with the process selected in step 2.
4. Change the value of the displayed parameter using key input if necessary.

■ In the nD Processor window

This method explains using an example of replacing the process list in two-dimensional NMR data.

1. Click on the **Change** button in the **nD Processor** window to make **Change** mode.
2. Click on the **X** or **Y** button to select the axis in which the process is to be replaced.
   X: When adding the process to the X-axis (direct observation axis).
   Y: When adding the process to the Y-axis (indirect observation axis).



3. Select the process to replace in the process list.
4. Select the process to replace from the data-processing button or the menu bar.
   The process selected here is replaced with the process selected in step 3.
5. Change the value of the displayed parameter by key input if necessary.

1.4.3d Moving the process

This section explains how to move the process specified in the process list.

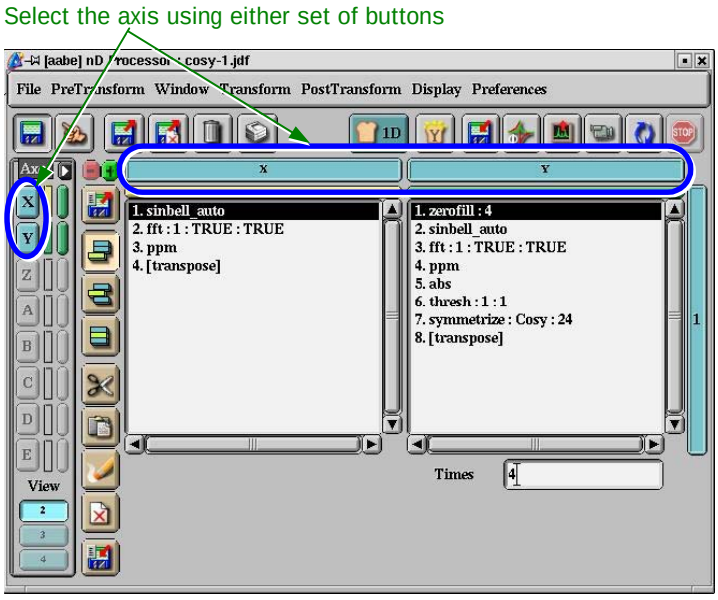
In the 1D Processor window

1. Select the process to move in the process list.
2. Click on the **Cut** button.
   The selected process is deleted.
3. Select the process to be performed after the process you are moving in the process list.
4. Click on the **Paste** button.
   The process you are moving is inserted before the process selected in step 3.

In the nD Processor window

This method is explained using an example of moving the process list in the two-dimensional NMR data.

1. Click on the **X** or **Y** button to select the axis which moves the process.
   X: When adding the process to the X-axis (direct observation axis).
   Y: When adding the process to the Y-axis (indirect observation axis).



2. Select the process to move in the process list.
3. Click on the **Cut** button.
   The selected process is deleted.
4. Select the process to be performed after the process you are moving in the process list.
5. Click on the **Paste** button.
   The process you are moving is inserted before the process selected in step 4.

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1.4.3e Deleting a selected process

This section explains how to delete a selected process.

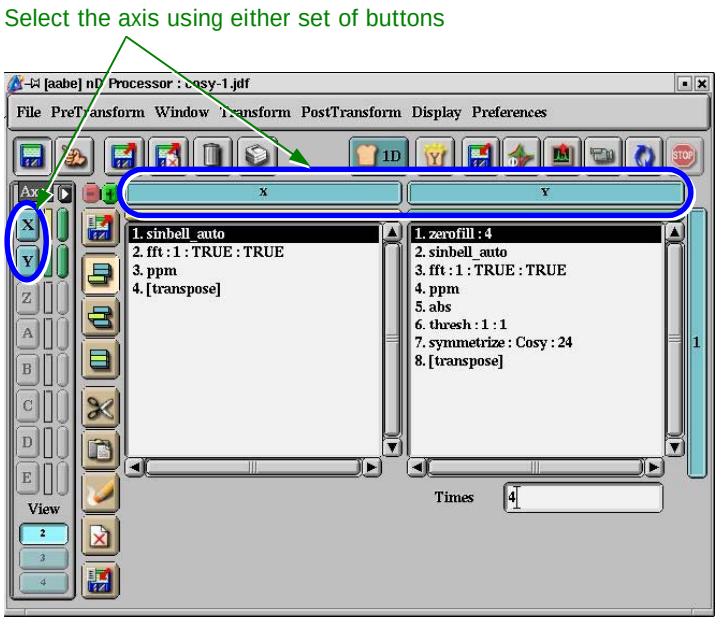
In the 1D Processor window

1. Select a process to delete in the process list.
2. Click on the **Delete** button.
   The selected process is deleted.

In the nD Processor window

This deletion method is explained using the process list of 2D NMR data as an example.

1. Click on the **X** or **Y** button to select the axis which deletes the process.
   X: When adding the process to the X-axis (direct observation axis).
   Y: When adding the process to the Y-axis (indirect observation axis).



2. Select the process to delete in the process list.
3. Click on the **Delete** button.
   The selected process is deleted.

1.4.3f Deleting all processes

This section explains how to delete all processes in the process list.

In the 1D Processor window

◆ Click on the **Clear** button.

All processes other than display/phase are deleted.

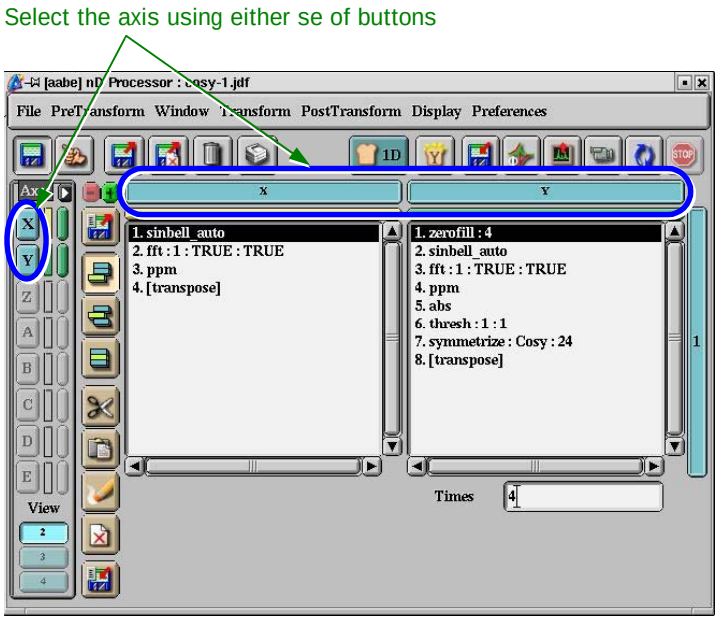
In the nD Processor window

This all deletion method is explained using the process list of two-dimensional NMR data as an example.

1. Click on the **X** or **Y** button to select the axis that deletes the process.

X: When adding the process to the X-axis (direct observation axis).

Y: When adding the process to the Y-axis (indirect observation axis).



2. Click on the **Clear** button.

All processes other than **transpose** are deleted.

3. Repeat steps 1-2 if necessary.

There is no function to delete the process list of all axes simultaneously. Delete a process list in each axis.

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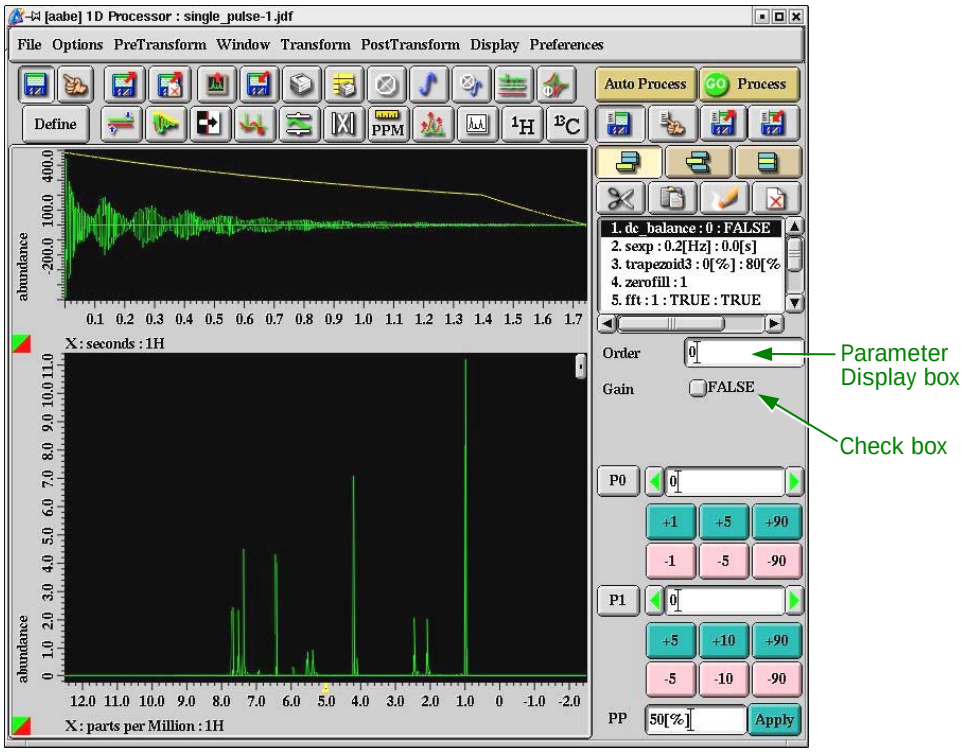
1.4.3g Changing process parameters

This section explains how to change the value of the parameter used in the process set up.

■ In the 1D Processor window

1. Select the process which changes a parameter in the process list.

The parameter used in the selected process and its value are displayed on the parameter display box or check box under the process list display area.



2. Change a parameter value in the parameter display box or the check box.

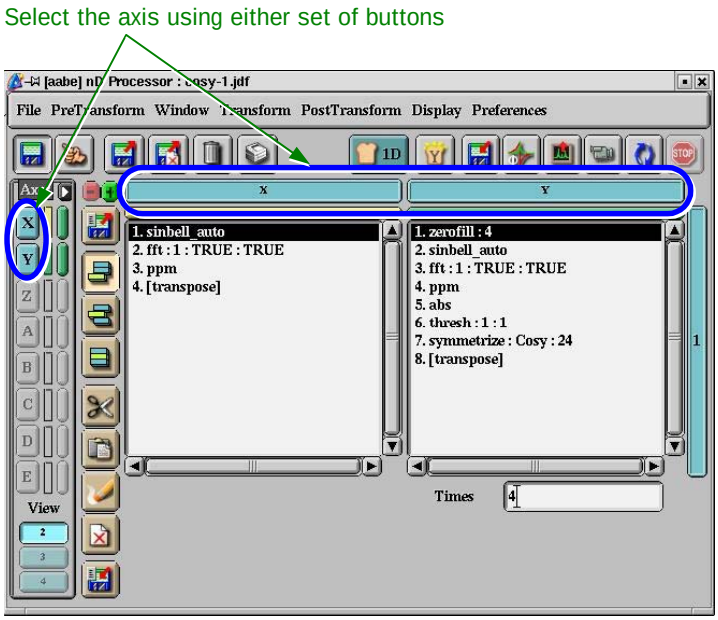
In the nD Processor window

This method for changing a process parameter in two-dimensional NMR follows.

1. Click on the **X** or **Y** button to select the axis in which a process will be changed.

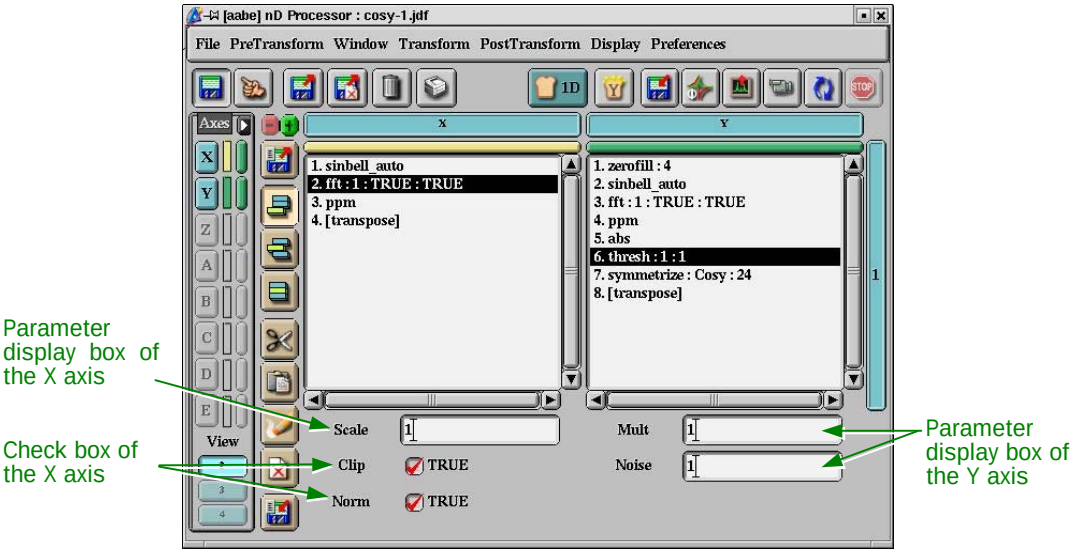
X: When adding the process to the X-axis (direct observation axis).

Y: When adding the process to the Y-axis (indirect observation axis).



2. Select the process which in the process list whose parameter you wish to change.

The parameter used in the selected process and its value are displayed on the parameter display box under process list display area.



3. Change parameter value in the parameter display box or the check box.

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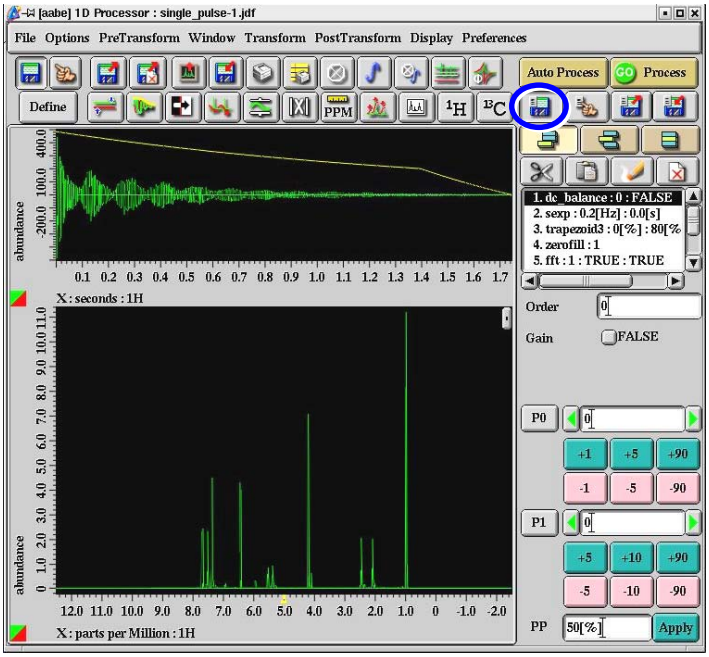
1.4.4 Reading in a Process List

To read the process list, there are two methods:

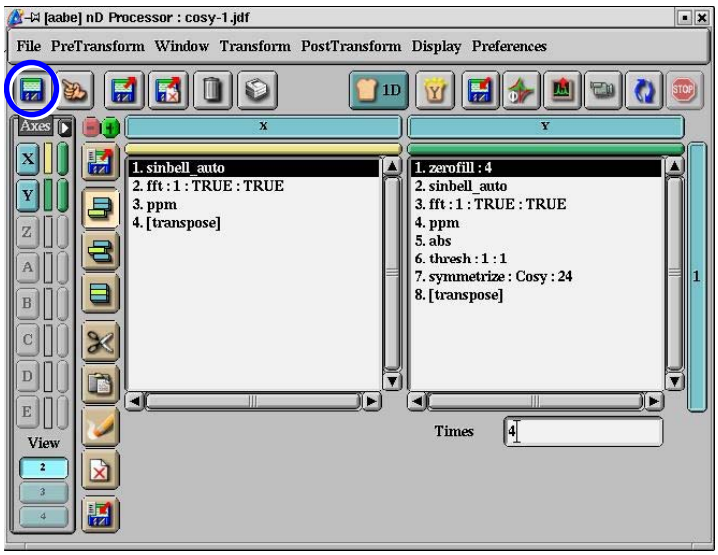
- Reading a process list file from hard disk.
- Reading a process list from another window displayed on the screen.

1.4.4a Reading the process list file from a disk

1. Click on the **Load List From Disk** button in the **1D Processor** window:



In the case of the **nD Processor** window, click on the **Open Data From Disk** button:



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2. Click on the **Open Processing List** button.
   The **Open Processing List** window opens :

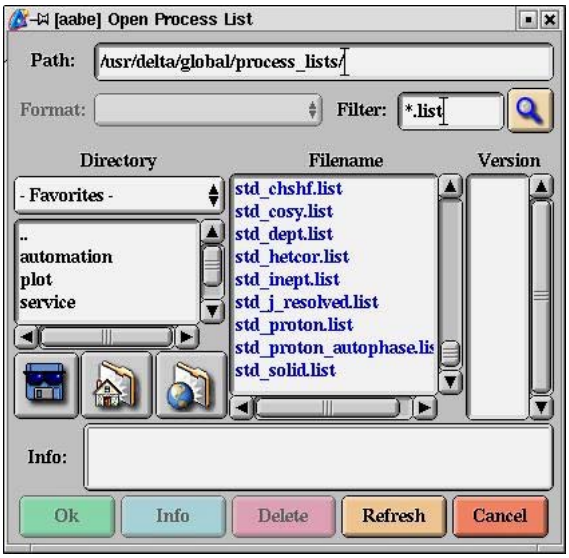

Fig. 1.11 Open Processing List window

3. Select the target process list from the process lists.

4. Click on the Ok button.
   The selected process list is read.

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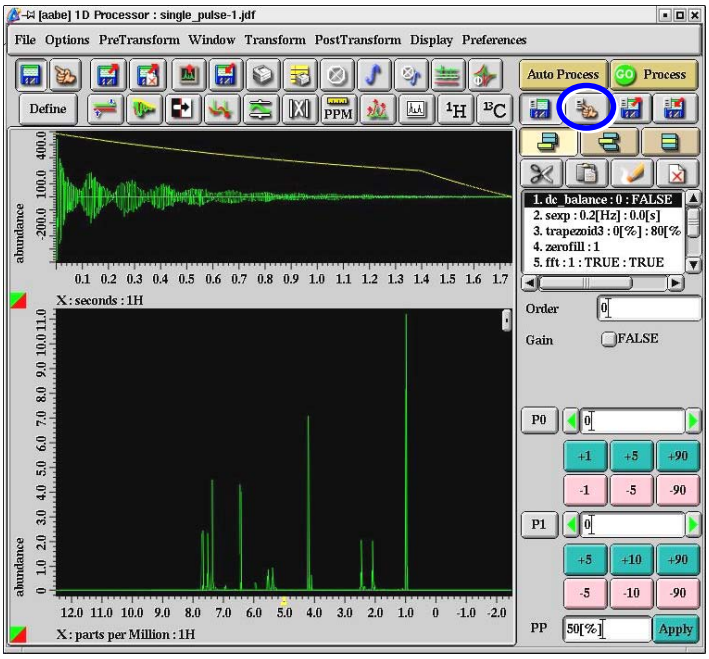
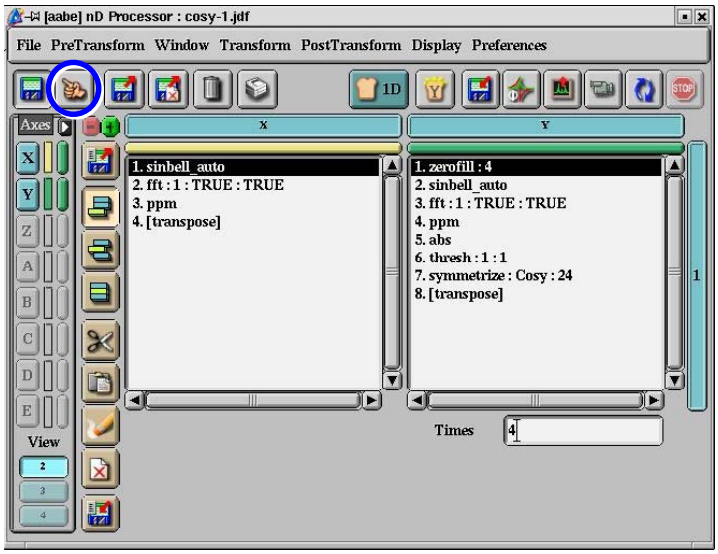
1.4.4b Reading from another window displayed on the screen

1. Click on the **Open List By Fingering Processor** button in the **1D Processor** window.



In case of the **nD Processor** window, click on the **Load List By Fingering Geometry** button.



2. Click on the **Open Processing List** button.

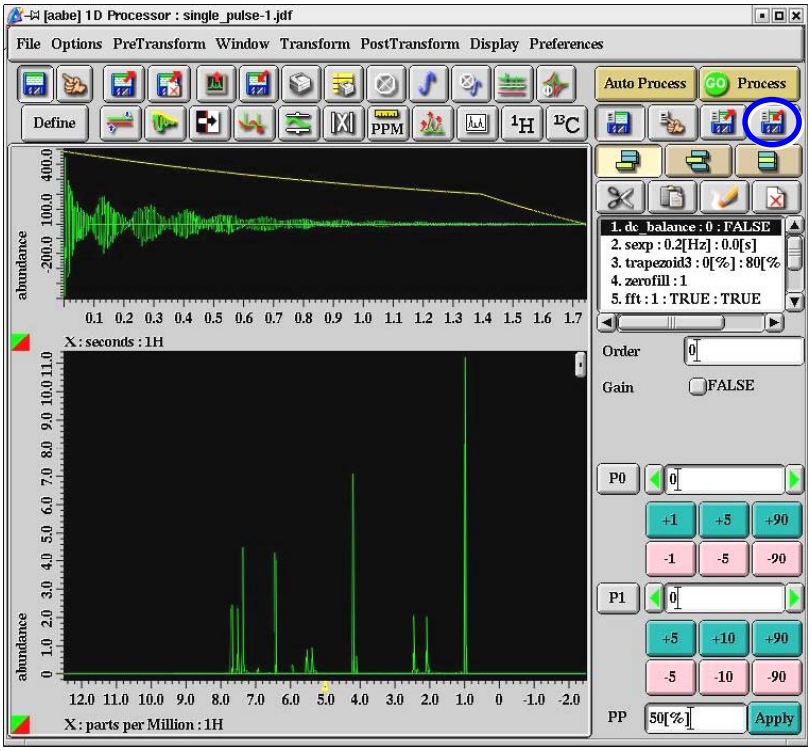
The mouse pointer changes to a finger.

3. Move the mouse pointer to the window in which the process list to set up is displayed, and click on the left mouse button.

The process list displayed on the specified window is read in.

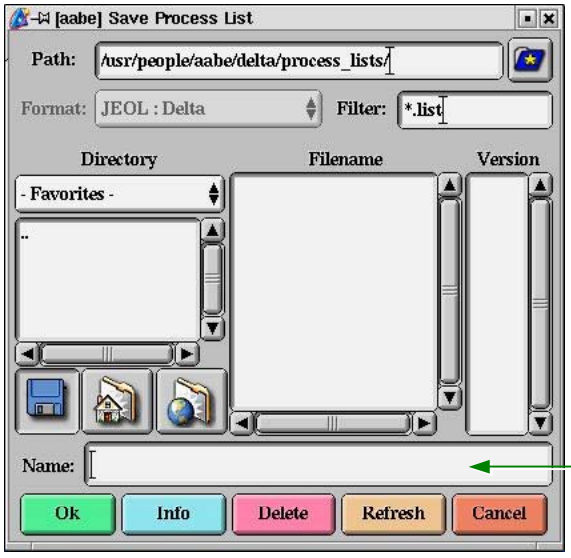
1.4.5 Saving a Process List

1. Click on the **Save Processing List To Disk** button.



The **Save Processing List** window opens.

2. Enter a file name in the file name input box.



When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

3. Click on the **Ok** button.

The contents of a process list are saved in a file.

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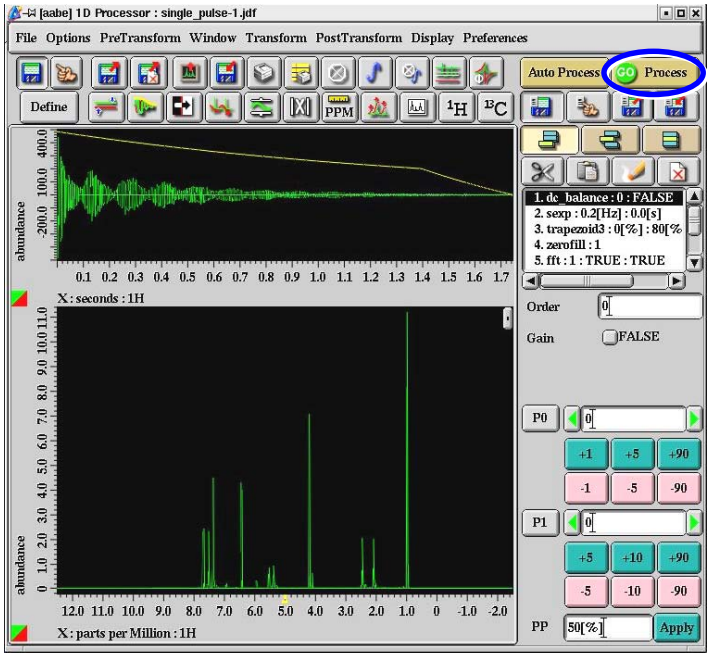
1.4.6 Executing a Process List

■ In 1D Processor window

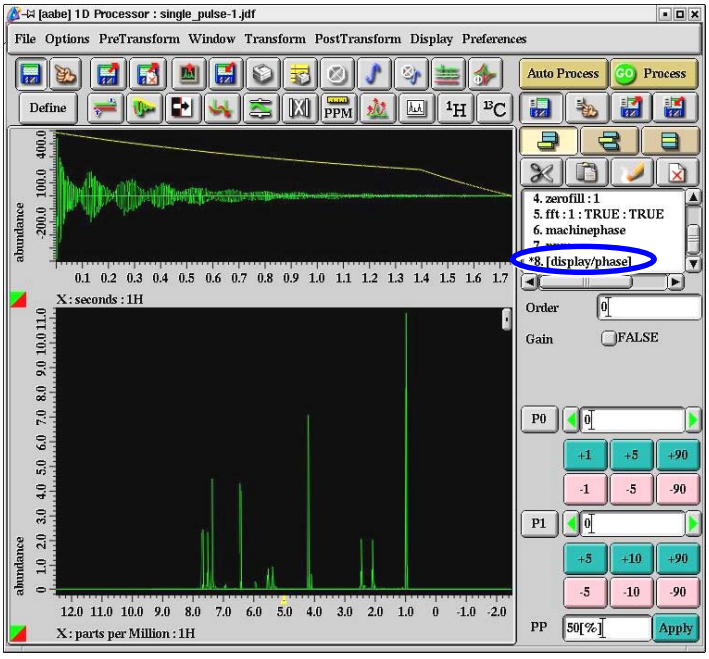
◆ Click on the **Process** button.



The **Process** button changes to an **Abort** display while executing a process list.
The spectrum in which the data processing of a process list is performed is displayed in the data display area.

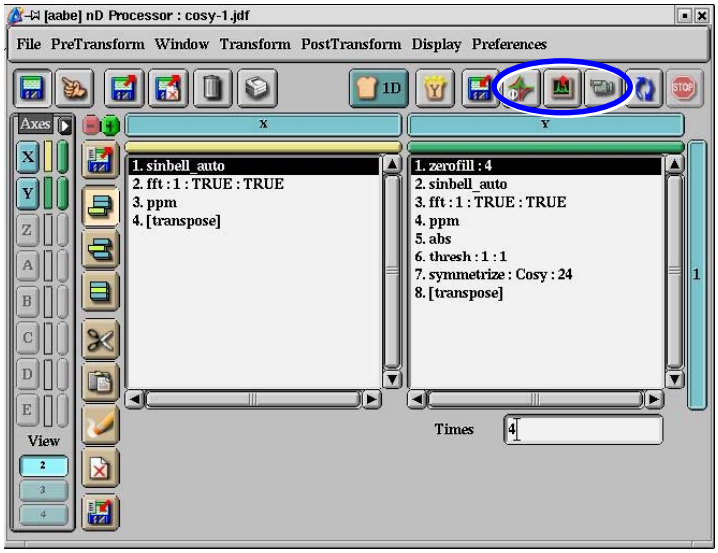
● Reference: Check that the process list has performed

When the * mark is displayed on the **display/phase** processing in the last item of the check process list, it shows that all processing in a process list has been performed.



In the case of the nD Processor window

- Click on the target button from the three buttons below:



Button	Button name	Explanation
	Process File and Put in a 2D Phaser	When the measurement data is two-dimensional phase sensitive detection data, the **Phase 2D** window appears after performing data the processing of a process list.
	Process File and Put In a Data Slate	After performing the data processing of a process list, the **Data Slate** window appears.
	Process File and Put In a Data Viewer	After performing the data processing of a process list, the **2D Viewer** window appears.

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1.5 READING AND SAVING DATA

This section explains how to read and save the data.

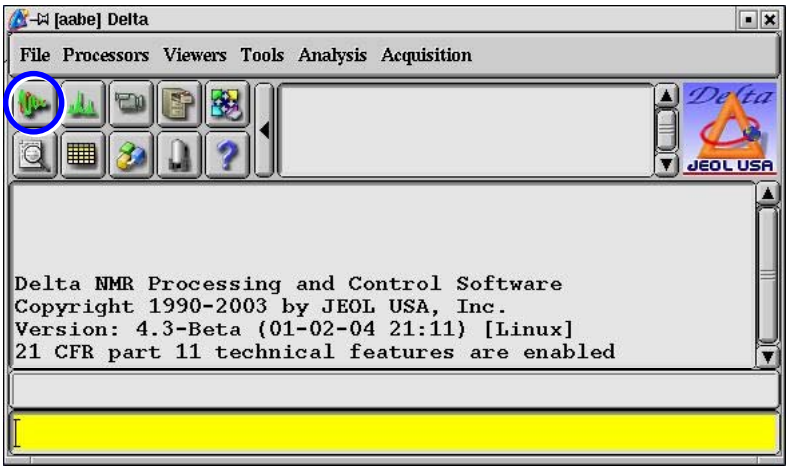
1.5.1 Reading Data

The data can be read in the following tool:

- **Data Processor**
- **Data Slate**
- **Data Viewer**

1.5.1a Reading data to a Data Processor

1. Click on the **Data Processor** button in the **Delta Console** window.


[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.
Version: 4.3-Beta (01-02-04 21:11) [Linux]
21 CFR part 11 technical features are enabled

The **Open Data for Processing** window opens.

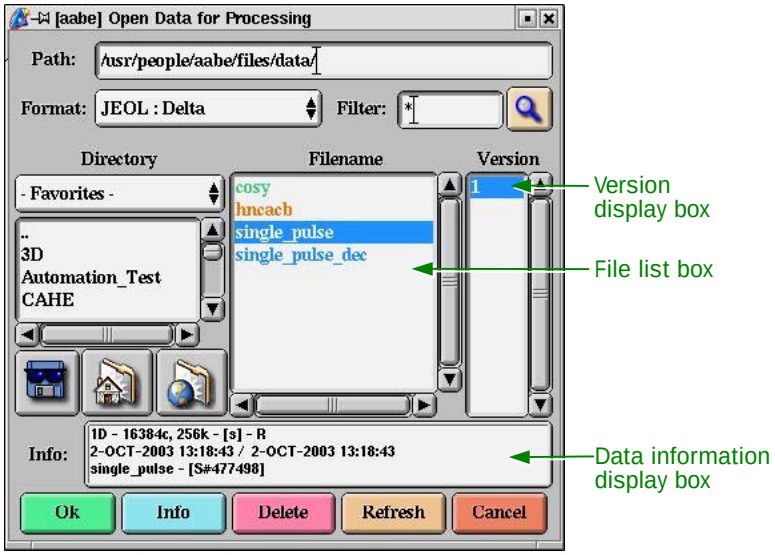
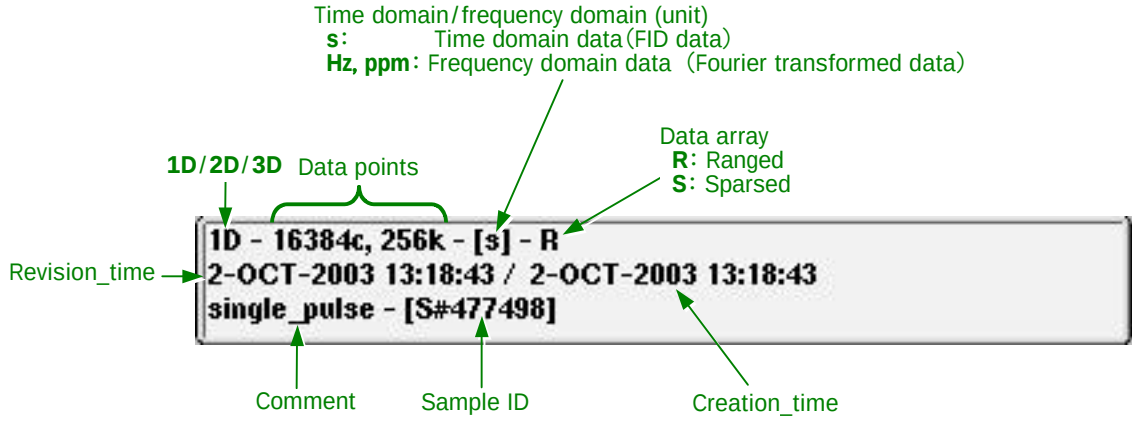


Fig. 1.12 Open Data for Processing window

2. If you specify the file name in the file list box and a version in the version display box, information will be displayed on the data display box; then verify the contents of a file to read.



3. Click on the **Ok** button.

In the case of one-dimensional data, the **1D Processor** window opens. In the case of multi-dimensional data, the **nD Processor** window opens.

■ Version number

The version of a file is supported by Delta.

On both sides of the hyphen "-", a version number is added behind a file name; ".jdf" of the file extension is appended next.

Before processing a data set, the file of a different version with the same file name as the original data is created automatically; the original data set is never processed. Therefore, have no fear of destroying original data. If the user saves data using the same file name, version number may become large. Because data may also be deleted after using the copied data for processing, it is also common for the version number of the listed file is discontinuous.

✍ When a file version is not selected in the **Open Data for 1D Processor** window, the data of the newest version (that has the largest number) is read.

■ Directory

Although selection of a local directory and a global directory can be performed in the **Open Data for 1D Processor** window, the user uses the local directory. The global directory is write inhibited.

If you click on the button, the file list of local directories appears on the file list box in the **Open Data for 1D Processor** window.

✍ The local directory is specified to **DATA** of the **.delta_configure** file.

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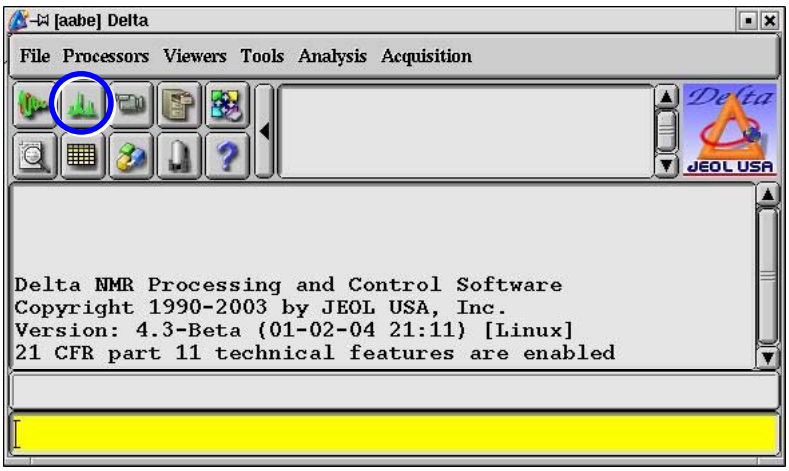
1.5.1b Reading data to a Data Slate

This section shows how to read processed one-dimensional NMR data finished data processing into a **Data Slate**.

1. Click on the **Data Slate** button in the **Delta Console** window.


[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.
Version: 4.3-Beta (01-02-04 21:11) [Linux]
21 CFR part 11 technical features are enabled

The **Open Data for Data Slate** window opens.

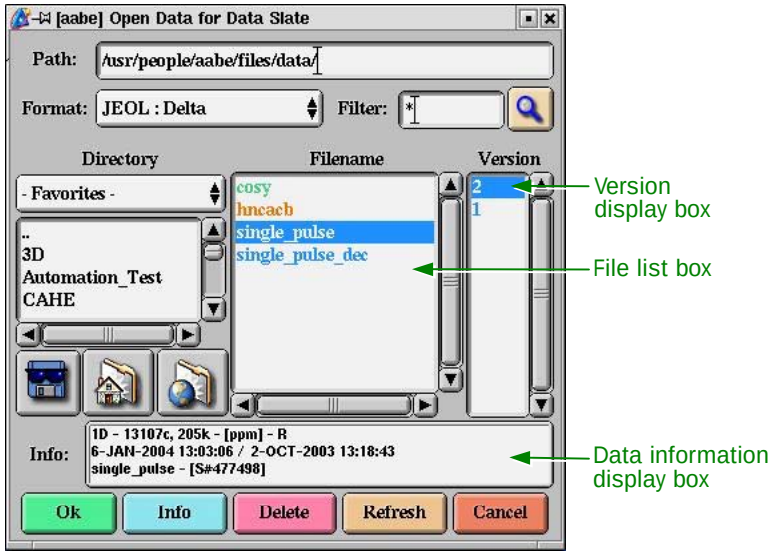


Fig. 1.13 Open Data for Data Slate Window

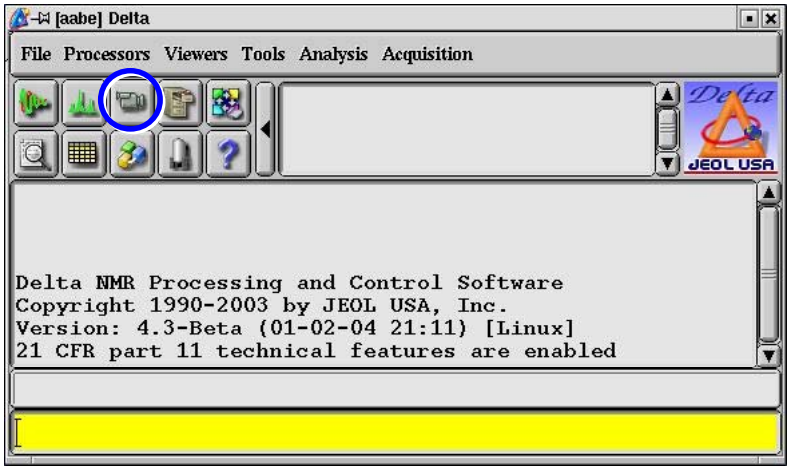
2. If you specify the file name in the file list box and a version in the version display box, information will be displayed on the data display box. Verify the contents of a file to be read.

3. Click on the **Ok** button.
The **Data Slate** window opens.

1.5.1c Reading data to Data Viewer

This section explains how to read processed two-dimensional NMR data finished data processing into **2D Viewer**

1. Click on the **Data Viewer** button in the **Delta Console** window.


[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.
Version: 4.3-Beta (01-02-04 21:11) [Linux]
21 CFR part 11 technical features are enabled

The **Open Data for Viewing** window opens.

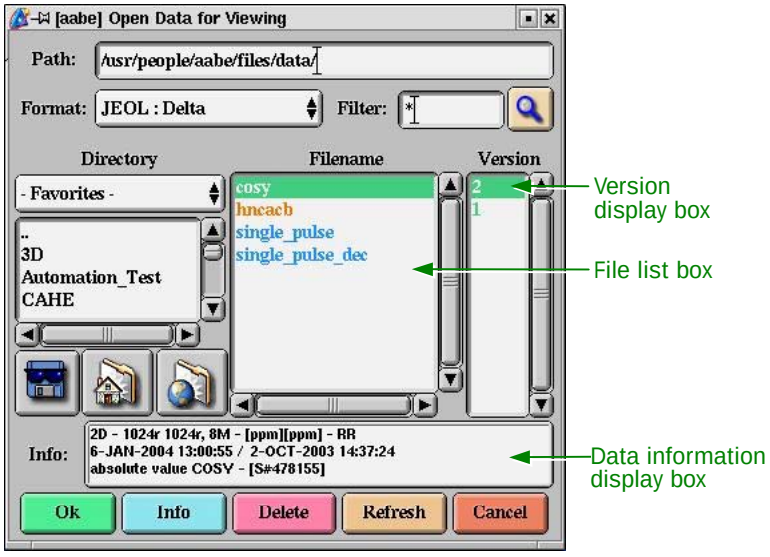


Fig. 1.14 Open Data for Viewing window

2. If you specify the file name in the file list box and a version in the version display box, information will be displayed on the data display box. Verify the contents of a file to be read.

3. Click on the **Ok** button.

The **2D Viewer** window opens.

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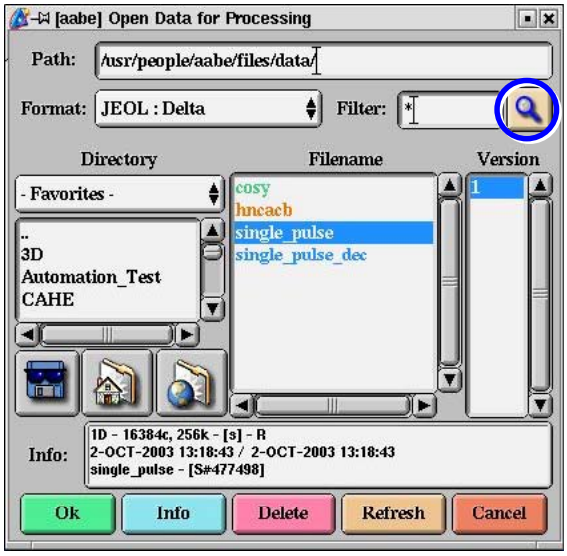
1.5.1d How to search for data

The **Open Data for Processing** window provides the **File Search** function, and can search for measurement data or a processing data with various conditions.

■ Search procedure

1. Click on the **Search for Files** button in the **Open Data for Processing** window.



The **File Search** window opens.

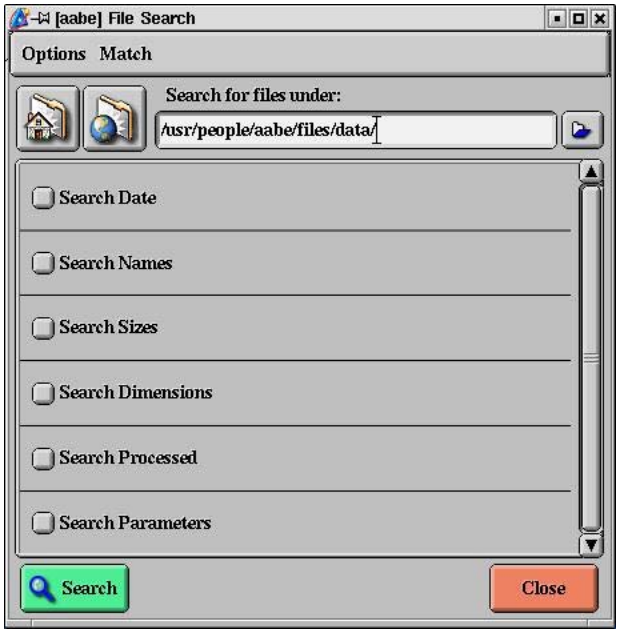
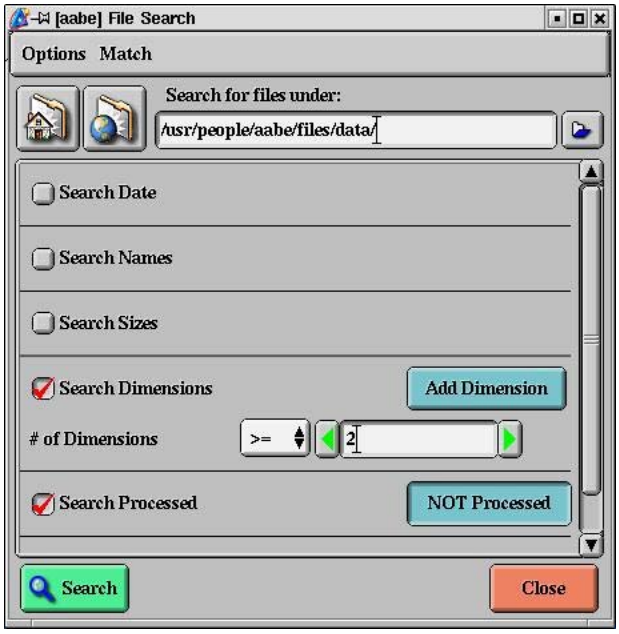


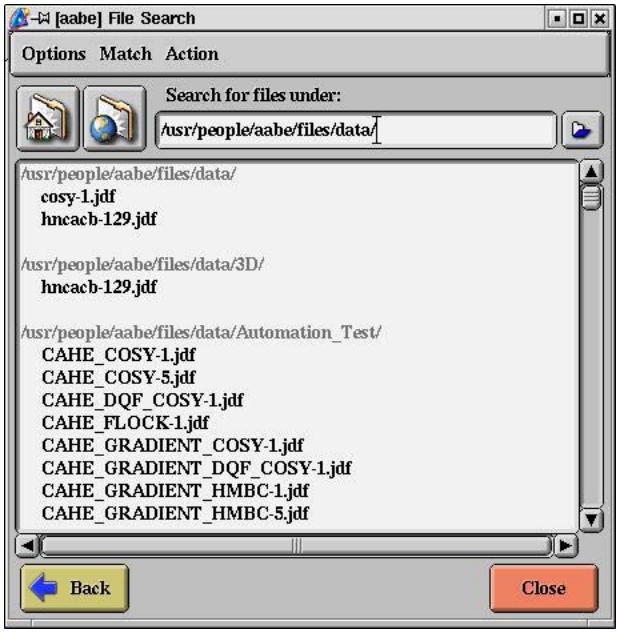
Fig. 1.15 File Search Window

2. Specify search conditions.

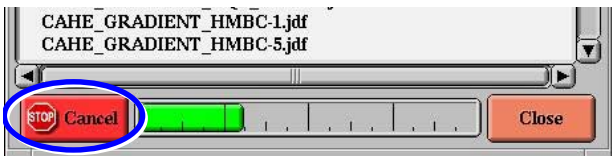
Date, file name, data size, number of dimensions, existence of processing and parameters can be specified to search conditions, respectively.
Moreover, two or more conditions can be specified simultaneously.



3. Click on the Search **Search** button.
A search result appears.



✍ In order to stop a search of a file on the way, click on the **Cancel** button displayed during the search.



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4. Click on the target file to select.

The processing button is displayed at the bottom of the window.

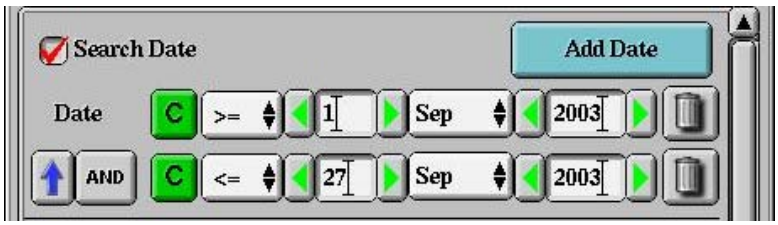
Button	Explanation
Back	Returns to search condition specification.
Select	Selects a file in the **Open for...** window.
	Opens a file in the **Data Processor** window.
	Opens a file in the **Data Slate** window.
	Opens a file in the **Data Viewer** window.
	Displays the parameter of a file in the **Parameter Viewer** window.

5. Click on the desired processing button.

The window opens according to the clicked processing button.

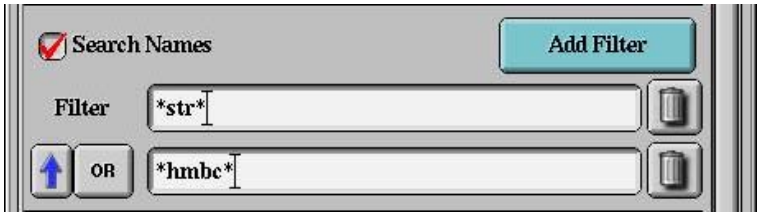
Search condition

Date



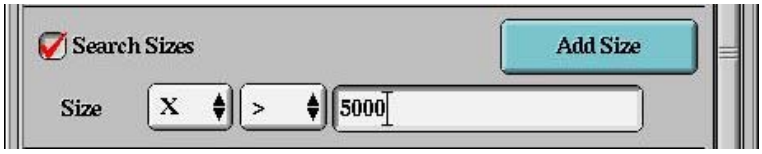
A file is searched for by the time stump attached to the file. The time stamp is the time stamp of an operating system, **Creation Date** C of a file, or **Revision Date** R of a file.
Data created between September 1, 2003 and September 27, 2003 is searched for in this example.

File name



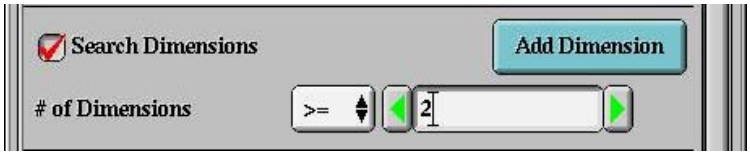
The data is searched for using a file name. A wild card "*" can be used.
Data which contains **str** or **hmbc** is contained in its file name is searched for in this example.

Data size



The data is searched for using the number of points of each observation axis.
Data whose the X-axis is smaller than 5000 points is searched for in the example in this figure.

A number of dimensions



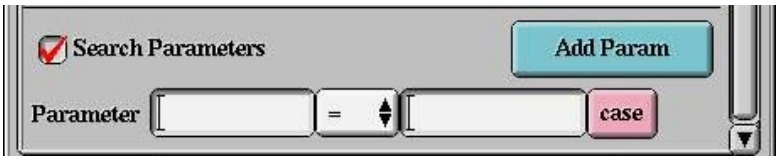
Data is searched for using the number of dimensions for a data.
Data more of than two dimensions is searched for in this example.

C I

Existence of processing

The data is searched for by measurement (FID) or processed data.
If you click on **Processed,** it will change to **Not Processed** and only the FID will be searched.

Parameter



Arbitrary parameters are made into search conditions.
All the parameters recorded in the Delta file, such as the number of scans to accumulate or kind of solvent, can be used for a data search.

1.5.2 Saving NMR data

This section explains how to save a data.

1.5.2a Saving measurement data

The measurement data (FID) is automatically saved by file name assigned in **filename** of the **Experiment Tool** window.

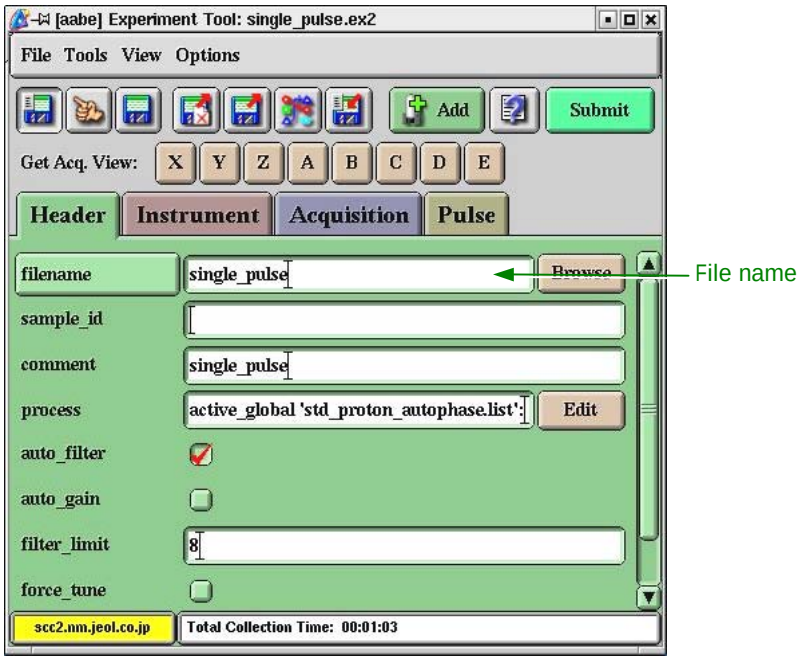


Fig. 1.16 Experiment Tool window

When measuring as is without changing the file name set in **filename**, the newest measurement data (FID) is saved by the same file name one version higher,
Change the data to another file name using the following operation when you want to change a file name after a measurement.

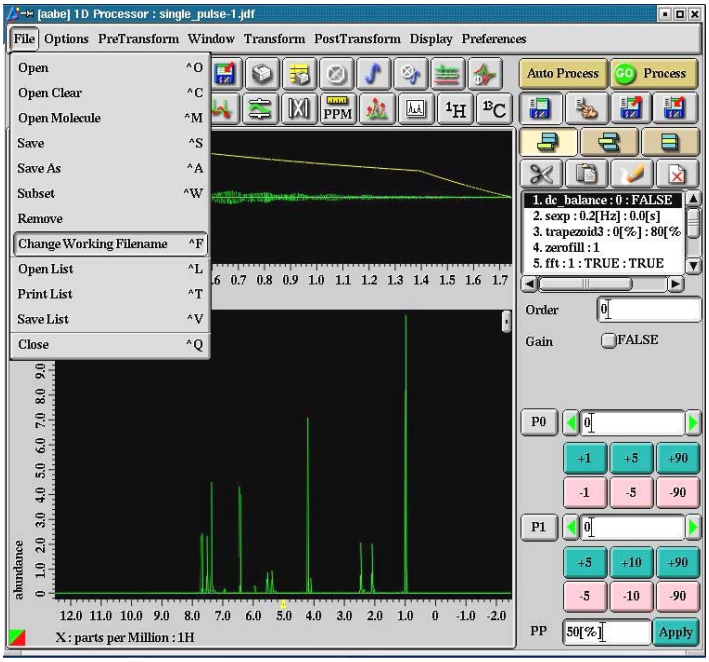
✍ Data is saved to the local data directory (usually ~/files/data).

C I

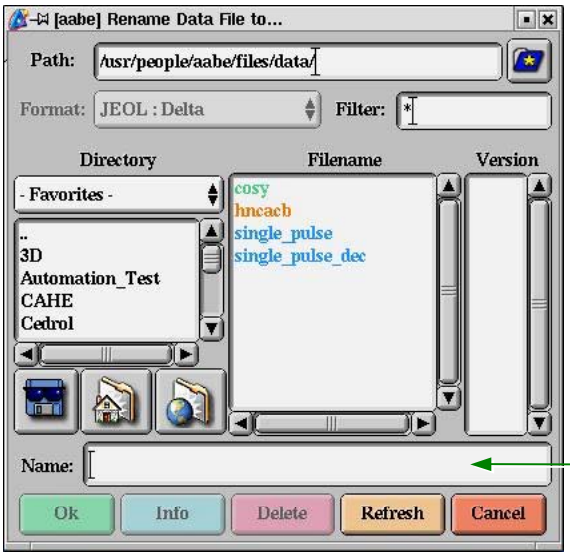
Changing the file name after measurement

A file name is saved in the following procedure in the state where the data to save is displayed on the **1D Processor** or **nD Processor** window.

1. Select **File–Change Working File** name in the **1D Processor** or **nD Processor** window.



The **Rename Data File to ...** window opens.



2. Input any file name in the file name input box using the key.

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

3. Click on the **Ok** button.

The measurement data is changed to the newly specified file name.

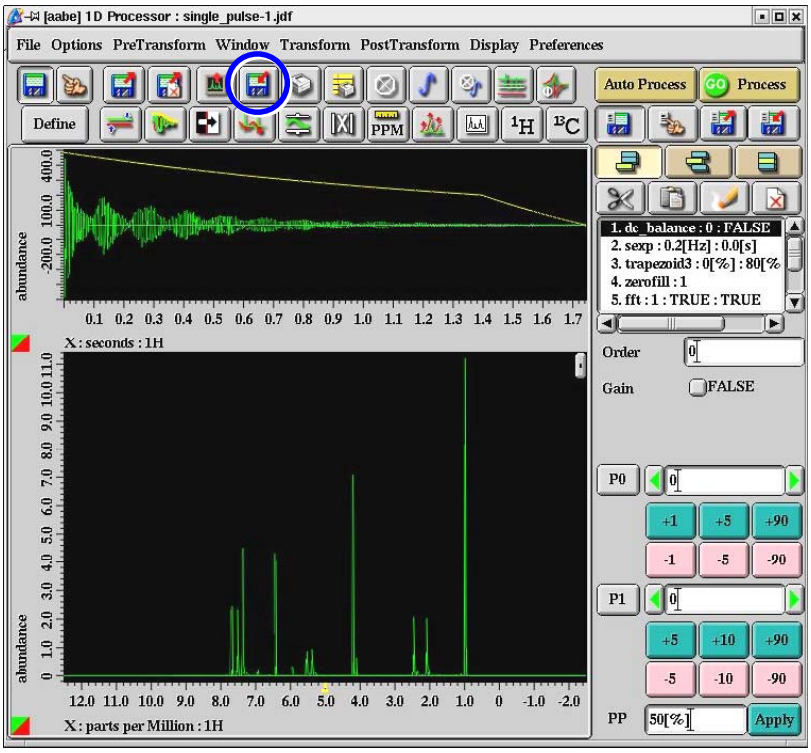
When a file by the same name already exists, the version number is raised by one.

1.5.2b Saving processing data

■ Saving 1D NMR data in the 1D Processor window

● When saving the data with the same file name

◆ Click on the **Save Processed Data to Disk** button in the **1D Processor** window.

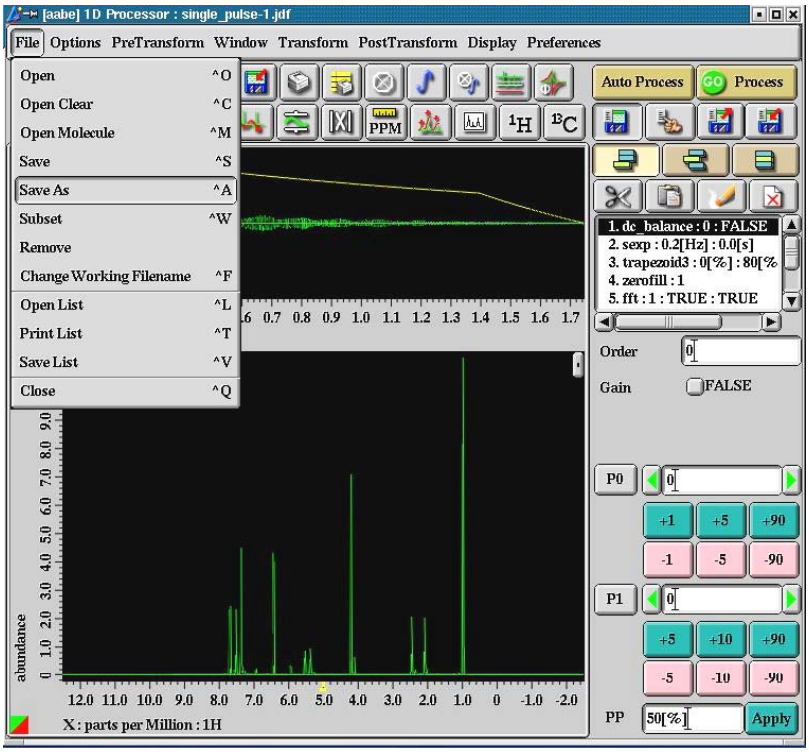


The1D processing data is saved. At this time, the version number automatically increases for the same file name.

C I

- **When saving the data to an other file name**

Select **File**–**Save As** in the menu bar of the **1D Processor** window.



The **Save Data File** window opens.

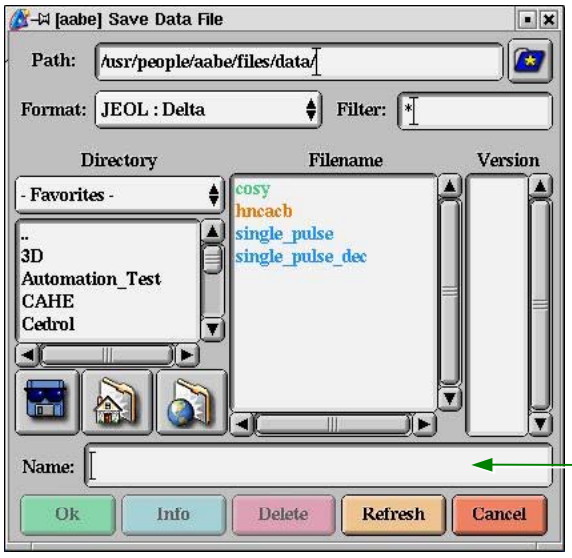


Fig. 1.17 Save Data File window

2. Enter any file name in the file name input box using the key.

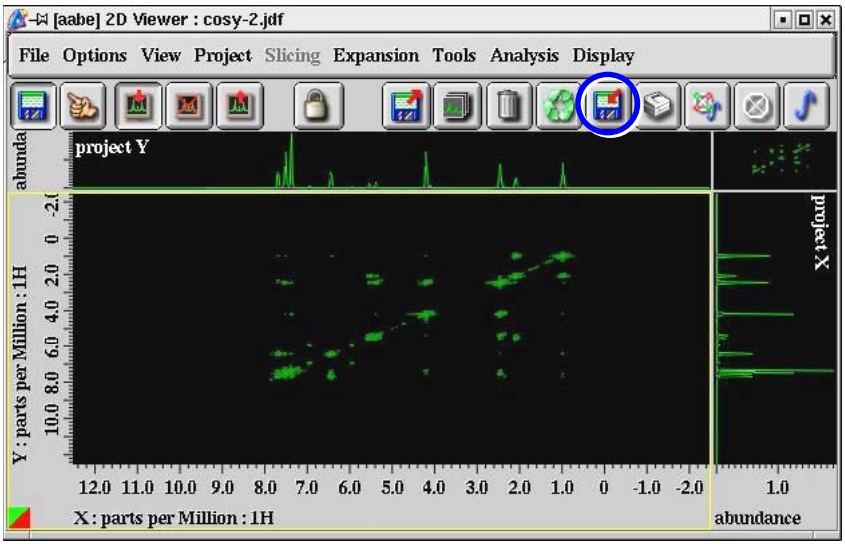
3. Click on the **Ok** button.

1D processing data is saved to the newly specified file name.

Saving 2D NMR data in the 2D2 Viewer window

When saving the data with the same file name

- Click on the **Save Currently Selected Data To Disk** button in the **2D Viewer** window.

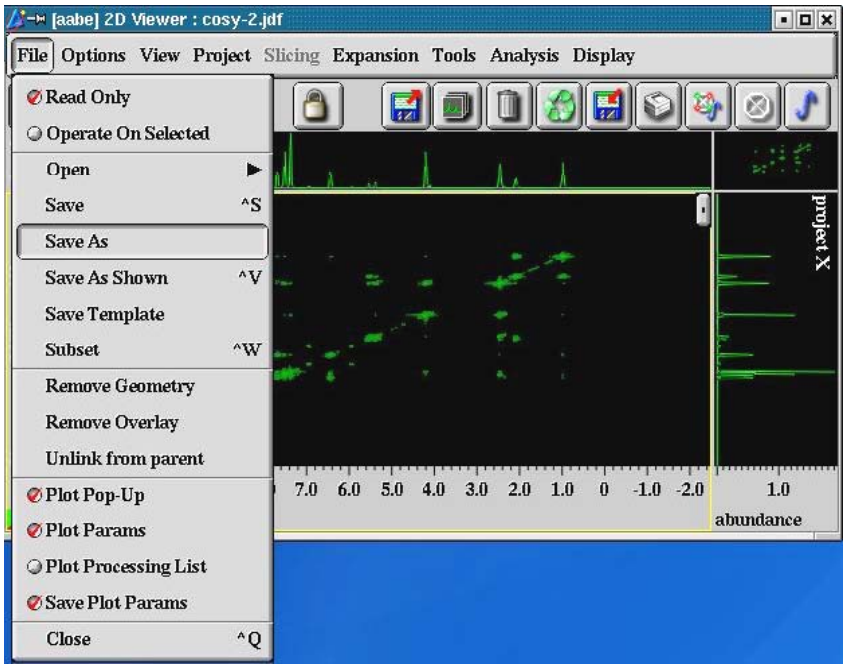

[aabe] 2D Viewer : cosy-2.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
project X
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

The 2D processing data is saved. At this time, the version number automatically increases for the same file name.

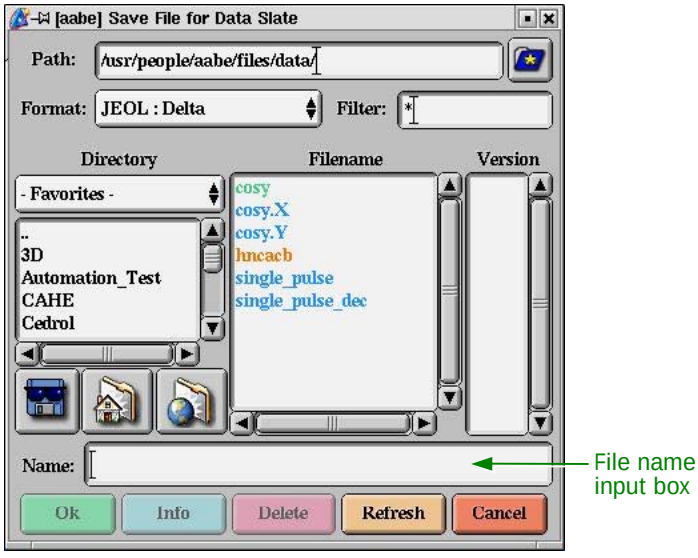
C I

- **When saving the data to an other file name.**

1. Select **File**–**Save As** in the menu bar of the **2D Viewer** window.



The **Save File for 2D Viewer** window opens.



2. Enter any file name to the file name input box using the key.

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

3. Click on the **Ok** button.

The 2D processing data is saved to the newly specified file name.

1.6 NMR DATA CONVERSION

Delta can convert a data format. Here, the import method for a data other than Delta and the export method to data other than Delta are explained.

1.6.1 Supported Data Formats

The format supported by data conversion and their restrictions are shown in the following table:

To / Form	Delta	GX	Alice	Generic Bin/Int	Generic ASCII	Nuts	Galactic	Felix	Felix (Win)	NMR Pipe	JCAMP	SIMPSON
Delta	—	1	1	2	1	4	4	4	3	2	1	4
GX/GSX/EX	1	—	1	1	1	4	4	4	3	4	1	4
GX 2D Phase	5	—	5	5	—	5	5	5	3	5	5	5
ALPHA	6	1	1	6	1	4	4	4	3	7	1	4
Lambda	1	1	1	1	1	4	4	4	3	4	1	4
Alice	1	1	—	1	1	4	4	4	3	4	1	4
Generic	2	1	1	—	—	4	4	4	3	2	1	4
CMX	6	1	1	1	4	4	4	4	3	4	4	4
Nuts	4	4	4	4	4	—	4	4	3	4	4	4
VXR/Unity	7	4	4	4	4	4	4	4	3	7	4	4
AC	8	8	8	8	4	8	8	8	3	8	8	4
AMX/DMX	2	1	1	2	1	4	4	4	3	4	4	4
Galactic	4	4	4	4	4	4	—	4	3	4	4	4
Felix	4	4	4	4	4	4	4	—	3	4	4	4
Felix(Win)	3	3	3	3	3	3	3	3	—	3	3	3
JCAMP	4	4	4	4	4	4	4	4	3	4	—	4
SIMPSON	4	4	4	4	4	4	4	4	3	4	4	—

Here, the numbers in the table refer to the following conditions.

Number	Conditions
1	1D, 2D(Absolute/Phase sensitive mode), Relaxation time
2	1D-4D
3	1D Only
4	1D, 2D(Absolute/Phase sensitive mode)
5	2D Phase sensitive mode
6	1D, 2D(Absolute/Phase sensitive mode), 3D(Absolute/Phase sensitive mode), Relaxation time
7	1D, 2D(Absolute/Phase sensitive mode), 3D(Absolute/Phase sensitive mode)
8	1D, 2D(Absolute)

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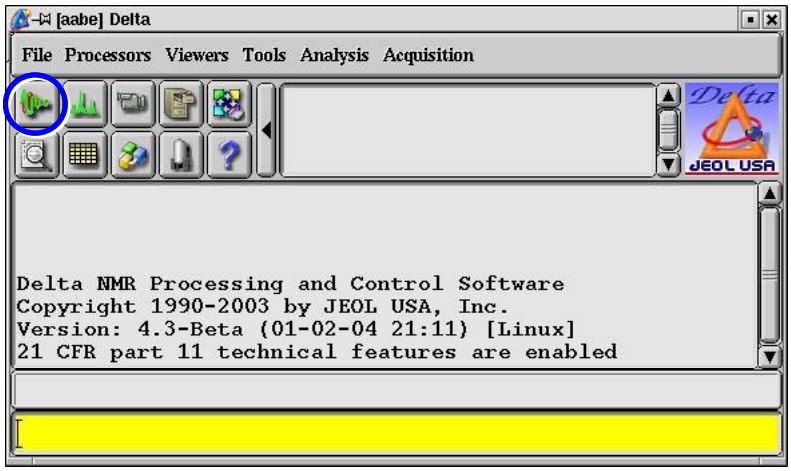
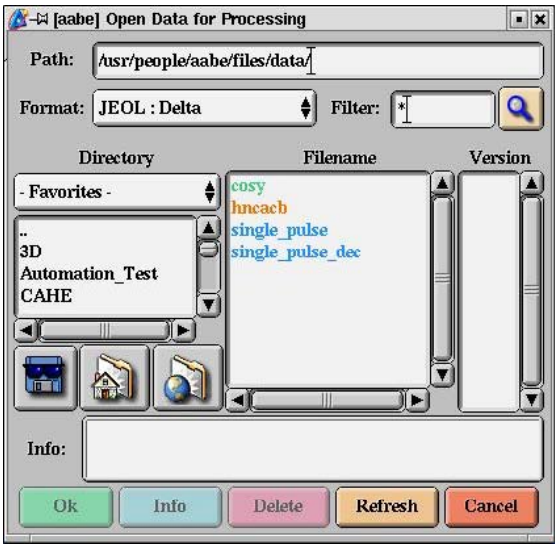
1.6.2 Importing Data

Importing data can be automatically performed at the time of reading in data.
Here, an example which imports and processes ALPHA 1D NMR data will be shown.

1. Click on the **Data Processor** button in the **Delta Console** window.


[aabe] Delta
File Processors Viewers Tools Analysis Acquisition
JEOL USA
Delta NMR Processing and Control Software
Copyright 1990-2003 by JEOL USA, Inc.
Version: 4.3-Beta (01-02-04 21:11) [Linux]
21 CFR part 11 technical features are enabled

The **Open Data for Processing** window opens.



2. Select **JEOL:Alpha** in the **Format** list.

3. Select **Foreign Data** in the **Directory** list.

✍ When the file is stored in directories other than **Foreign Data**, specify the directory of a storage place to **Path**.

4. Select the file displayed in the file name list displayed.

✍ Data information is not displayed on the data display box.

5. Click on the **Ok** button.

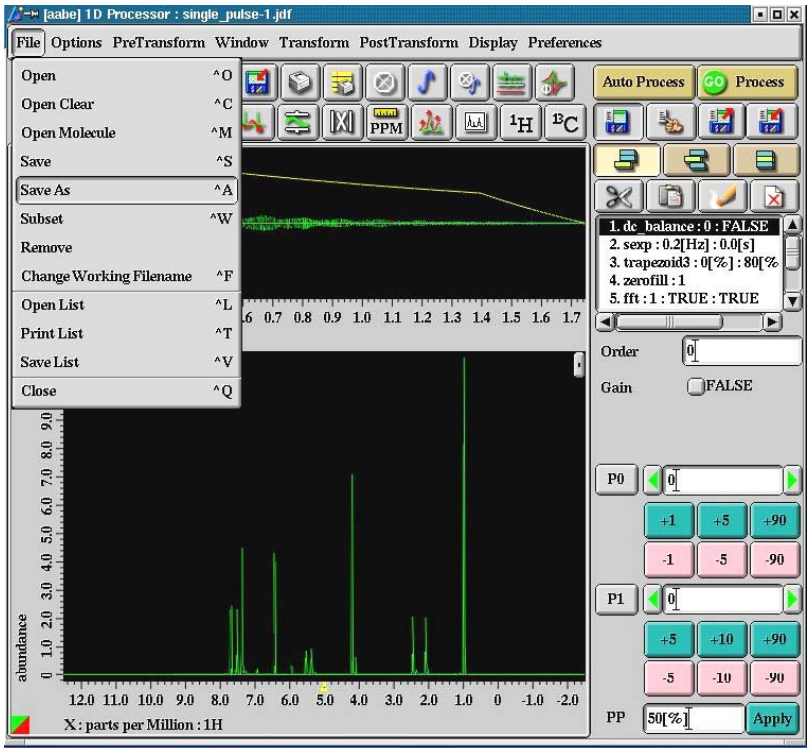
After performing automatic data import, the **1D Processor** window opens.

✍ Since there is no information in the process list, automatic setting of the process list cannot be performed.

1.6.3 Exporting Data

Exporting data can be automatically performed at the time of saving data.
Here, an example which exports and saves 1D NMR data to Alice will be shown.

1. Select **File**–**Save As** in the menu bar of the **1D Processor** window.



The **Save Data File** window opens.

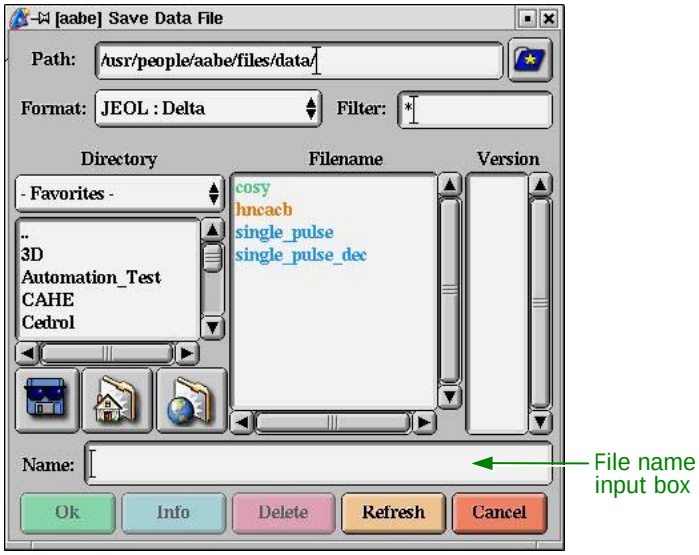


Fig. 1.18 Save Data File Window

2. Select **JEOL:Alice** in the **Format** list.

3. Select **Foreign Data** in the **Directory** list.

When storing a file to directories other than **Foreign Data**, specify the directory of the storage place to **Path**.

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4. Enter the arbitrary file name in the file name input box using the key.
5. Click on the **Ok** button.
   Exporting data is performed automatically and saved in a file.

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2

1D NMR DATA PROCESSING

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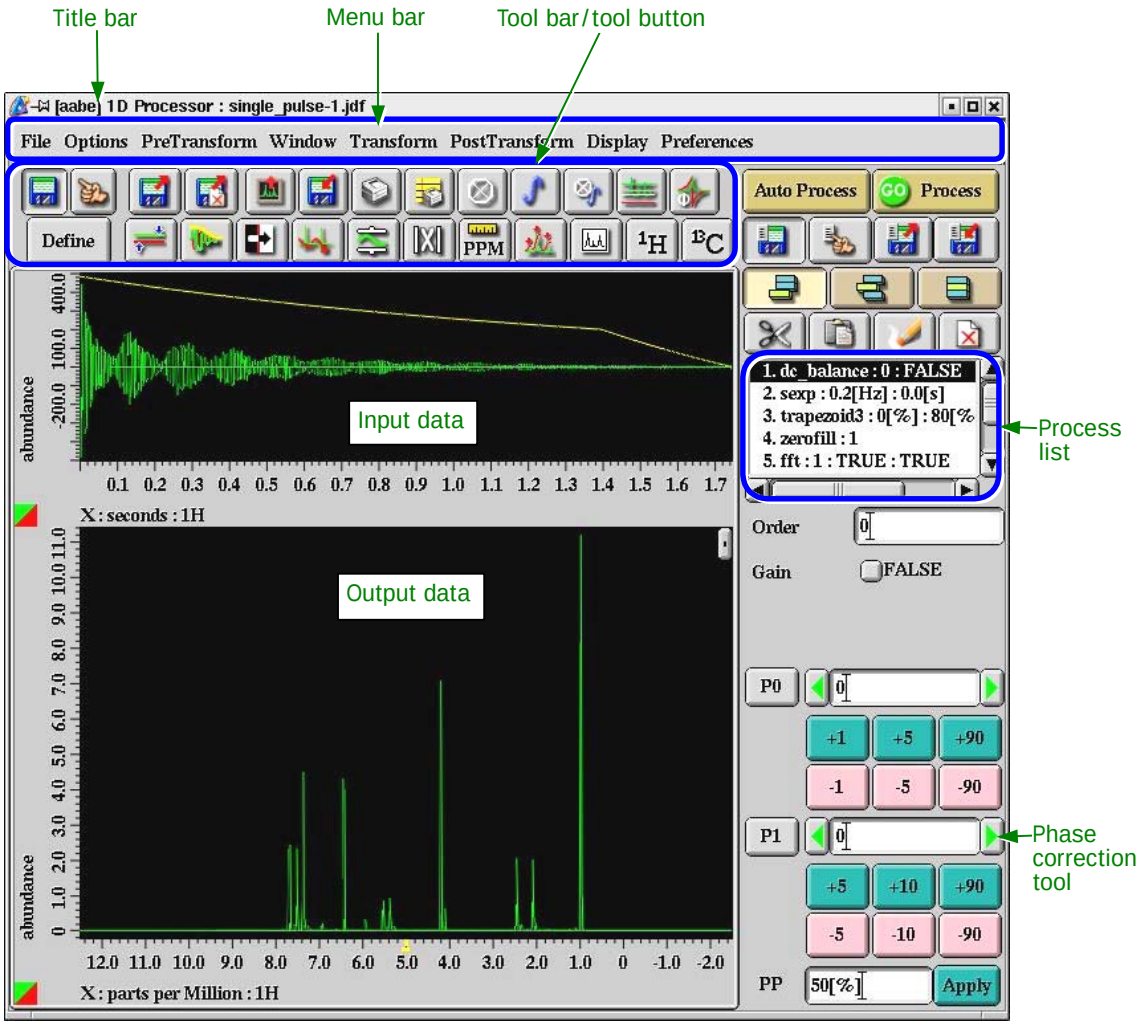
2.1 1D PROCESSOR WINDOW

In one-dimensional NMR data processing when data is read, the **1D Processor** window opens. Data processing is performed on this window.



The data file name is displayed on the title bar of the **1D Processor** window.
The **1D Processor** window consists of two display areas. The upper display area is an input domain, where the data before Fourier transform (the FID) is displayed. The lower display area is an output domain, where data is displayed after processing. The **process list** shows the data transformation methods used during data processing. Button and boxes for phase correction are displayed on the bottom right.

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Tool bar

In the tool bar on the upper part of the **1D Processor** window in extended mode, icons used for reading data files, storing processing data, a printing and automatic processing data are provided.

Button	Button name	Explanation
	Load List from Disk	Reads data from a hard disk.
	Finger	Reads data from an open window. For example, when reading data from window B to window A, first select the button in window A. Next, click on the button to change the mouse pointer to a finger. Move the mouse pointer to the B window and click on the data to move it. This is the reverse logic to the cut & paste function.
	Open File	Reads new data into the **1D Processor** window opened. If there is an already process list set-up, the contents are adapted immediately for the read data.
	Open Clear	Reads new data into the open**1D Processor** window. The present process list is deleted at this time.
	Put Processed Data into Data Slate	Transfers the data from the open **1D Processor** window to the **Data Slate** window.
	Save Processed Data to Disk	Saves the processing data to a hard disk. The file name remains the same; the version number goes up.
	Print	Prints processed data.
	Generate Report	Prints the Spread Sheet including all peak information.
	Auto Peak Pick	Performs automatic peak picking.
	Auto Integrate	Performs automatic integration.
	Peak Pick and Integrate	Performs automatic peak picking and integration.
	Compute and Show Statistics	Calculates data statistics including the maximum and minimum values for the threshold, noise, baseline level of a, and peak intensity.
	Auto Phase Spectrum	Performs automatic spectrum correction.

Macro button

The default function most often used is assigned for each button. The user can change the function assigned or can also assign to a button a macro function suite to that user's needs.

Button	Button name	Explanation
	Define	This button is used when the default function of a macro button is changed, or an item assigned to a process list. Click on the macro button after clicking on the **Define** button first. When the **Define Macro** window opens, select the icon to define.
	DC Balance	Eliminates the zero frequency noise produced by any shift in the balance of the AD converter.
	Window Function	Applies a Hamming window function to FID data. Another window function can also be assigned to this button.
	FFT (Fast Fourier Transform)	Performs fast Fourier transformation (FFT) . The time domain data is transformed to the frequency domain data. Functions of **Hilbert**, **IFFT, MaxEnt**, and **Transpose** can also be assigned to this button.
	Auto Phase	Performs phase correction. The function of **MachinePhase** can also be assigned to this button.
	Base Correct	Performs baseline correction for the frequency domain spectrum. Functions like **Base Correct**, **IBase Correct**, and **DC Correct** can also be assigned to this button.
	Abs	Calculates the absolute value of the data.
	PPM	Change the unit of the data axis to ppm. This can replaced by the **Hertz** or **Auto Reference** function.
	Peak Pick/Integrate	Performs the peak picking. This can also be replaced by the functions **Integrate**, **Apply integral**, or **Print peak list**.
	Plot Spectrum	Prints a spectrum and its parameters.
	Proton	The process of DC Balance, Single Exponential, FFT, Machine Phase, and PPM are recorded by default with this user-defined macro.
	Carbon-13	The process of DC Balance, Single Exponential, FFT, Machine Phase, and PPM are recorded by the default with this user-defined macro.

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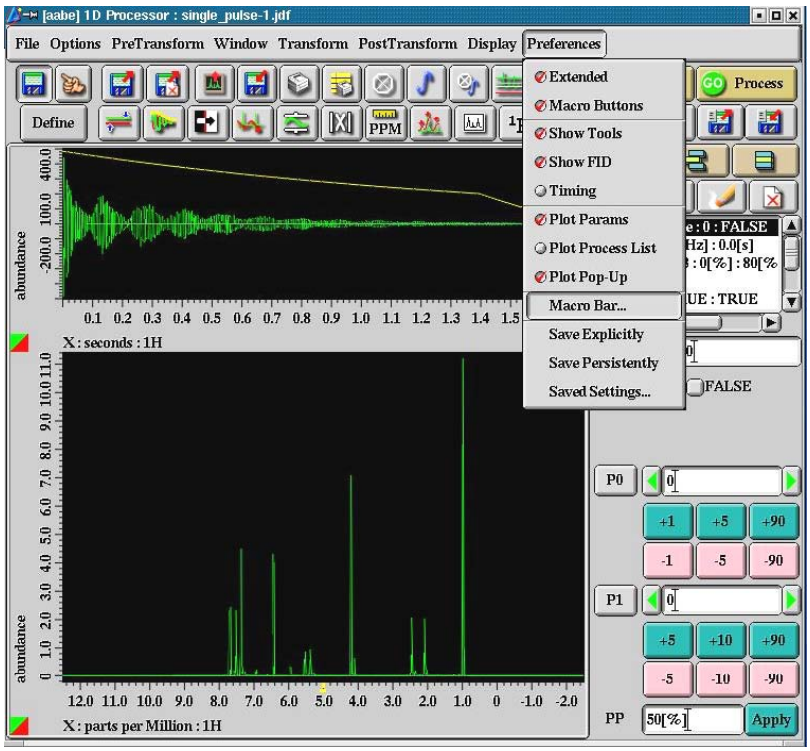
The macro button for the user

This is the button the user assigns to the macro for data processing.
It is assigned in the following procedure:

1. Select **Preferences–Macro Bar** from the menu bar in the **1D Processor** window.



The **Define Macro Bar** window opens.

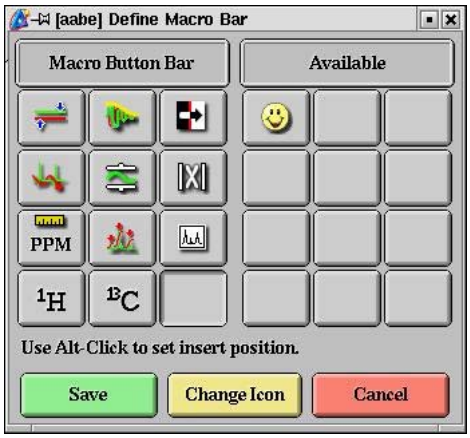


Fig. 2.1 Define Macro window

2. Select a macro button **Available** for users and click on the selected icon.
That icon is added to the **Macro Button Bar**.

3. Click on the **Save** button.
The new macro button will be added to the tool bar of the **1D Processor** window.

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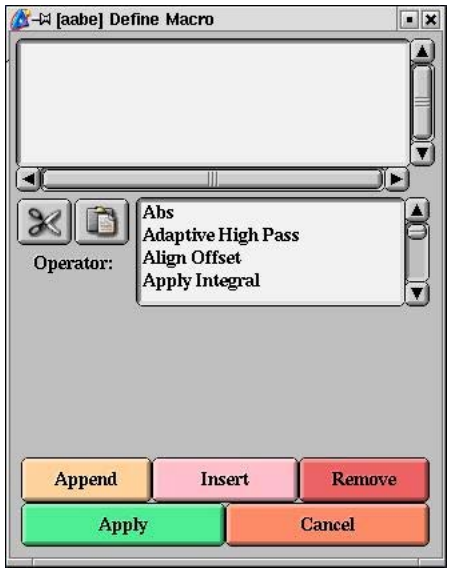
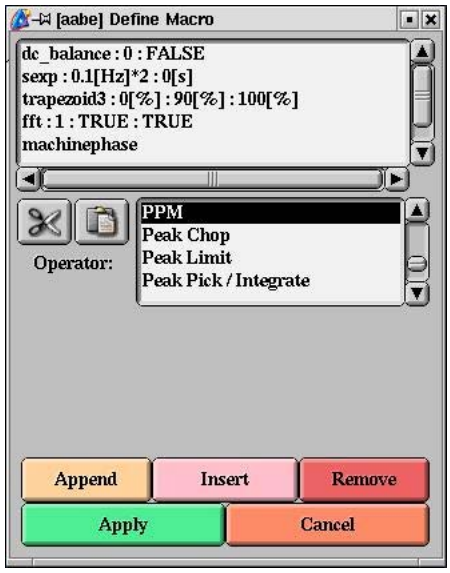
4. Click on the **Define** button in the **1D Processor** window, then click on the macro button added to the tool bar.

The **Define Macro** window opens.



5. Select the function to assign to the new button from the **Operator** menu, then click on the **Append** button.



6. Click on the **Apply** button.

The function selected in step 5 is assigned to the new macro button in the **1D Processor** window.

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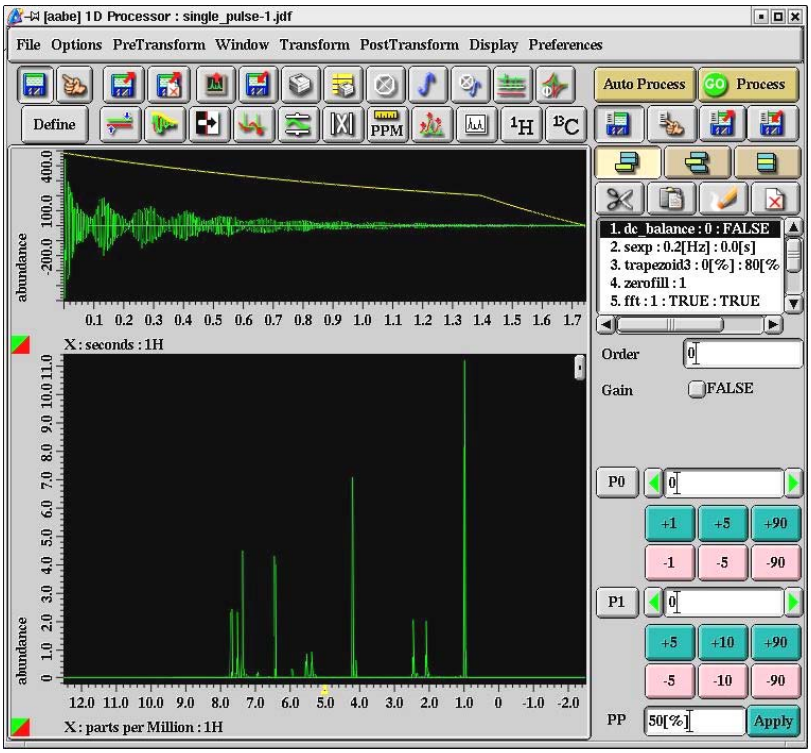
2.2 1D DATA PROCESSING

Data processing of one-dimensional NMR data is roughly divided into 5 processing steps:
These are

- Pre processing (data preparation before FFT
- Multiplication of Window function
- FFT
- Post processing (processing after FFT)
- Data display.

Each processing is classified and stored in the pulldown menu - **Pre Transform Window, Transform, Post Transform**, and **Display** in the tool bar of the **1D Processor** window. Data processing is performed combining these steps.

☞ Refer to the "Delta Programmer's Reference Guide" for details an each function.



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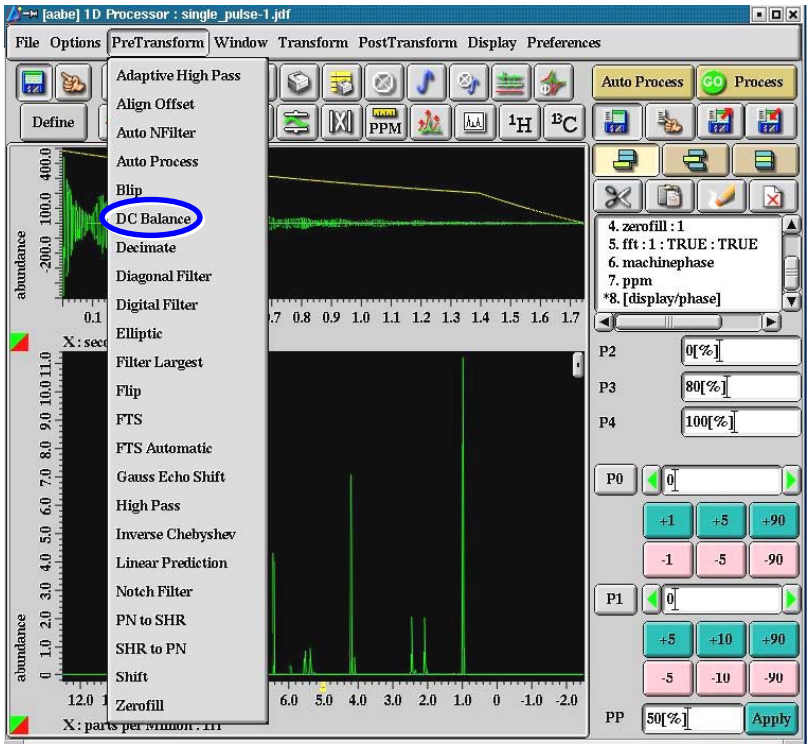
2.2.1 Canceling the DC Offset

The **DC Balance** function calculates the difference between DC offsets (constant) for the real and imaginary channels of the detector. DC offset causes "center spike noise" or "zero frequency noise" in data after Fourier transformation.

- Select **PreTransform–DC Balance** from the menu bar in the **1D Processor** window.



The **dc_balance** process is added to the process list.

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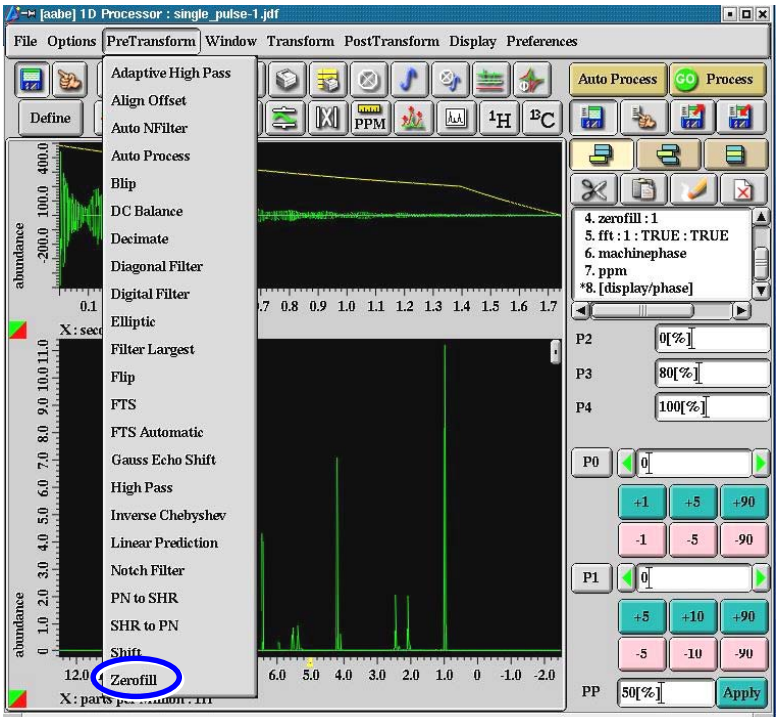
2.2.2 Zerofilling

The **Zerofill** function extends a data set by adding a specified number of zeros to the original data. Since the data size of every dimension consists of the *n*th power of 2, the specified number must be an *n*th power of 2 such as 1, 2, 4, 8, and 16.
If you enter a numerical value that is not an *n*th power of 2, the numerical value of the power of 2 larger than the entered value will be applied.

1. Select **PreTransform–DC Balance** from the menu bar in the **1D Processor** window.



The **zerofill** process will be added to the process list.
In zero filling, one argument is attached to the process. This argument is displayed in the **Times** input box.

2. Input the data scale factor.

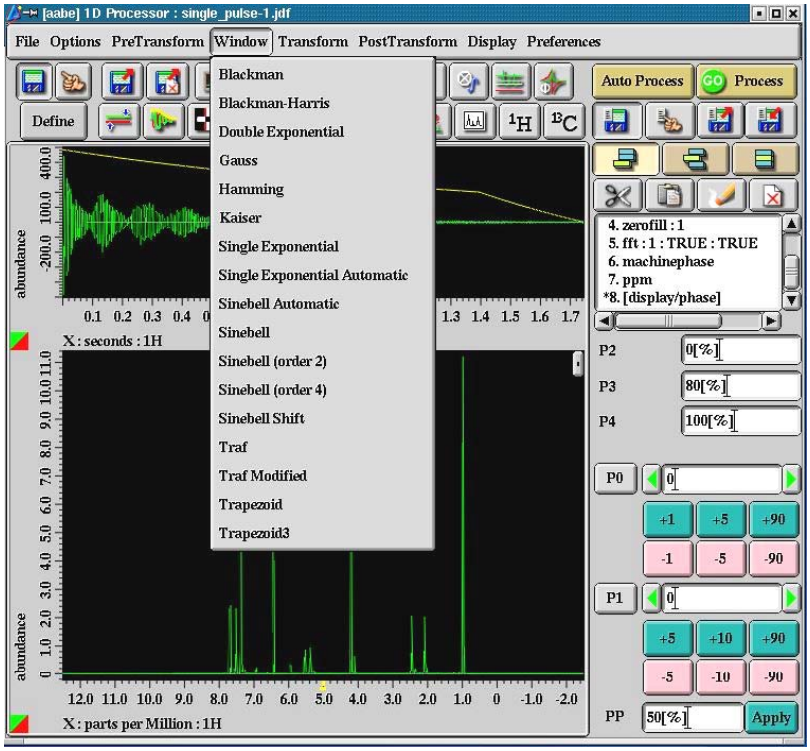
If 1 is entered in **Times**, zero filling is not performed to the data.

2.2.3 Window Function

The multiplication of a window function is used when emphasizing features, such as resolution enhancement and increasing the signal-to-noise ratio.

2.2.3a To set the window function:

1. Select arbitrary window functions from **Window** in the **1D Processor** menu bar.



The process you select will be added to the process list.
In a window function, arguments are often attached to the process. These arguments are displayed in the parameter input box.

2. Enter a parameter in the input box.

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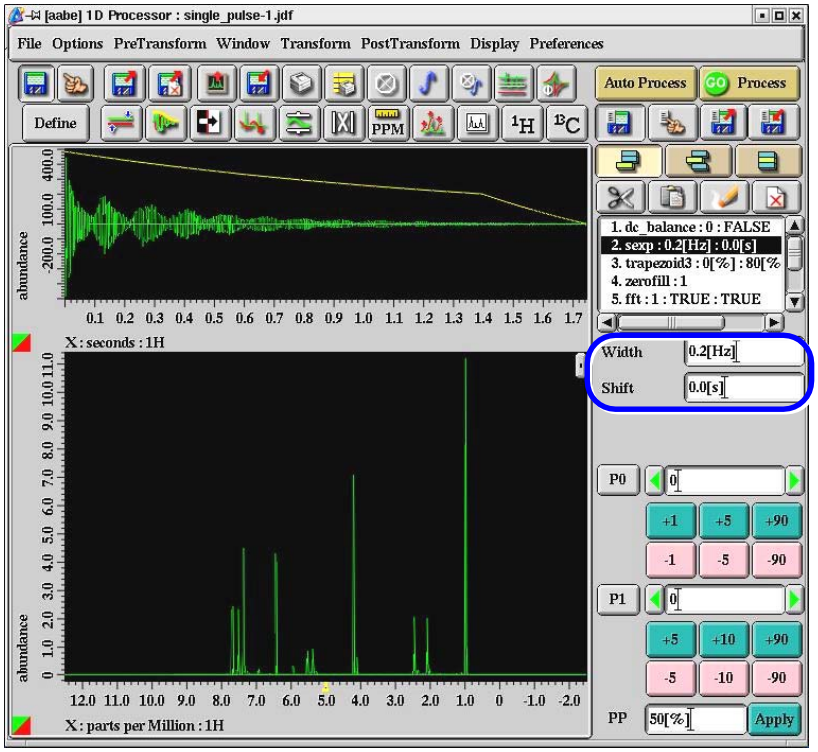
2.2.3b To change the parameters of the window function:

1. Select the window function from the process list.

The window function is highlighted.

An input box is displayed under the process list display area.



2. Key in any changes to the numerical value of the parameter for the displayed window function.

3. Click on the **Process** button.

The window function appears in the FID display area.

The spectrum re-processed using the window function with the changed value appears in the processing data display area.

4. Verify spectrum change.

5. Decide the optimum parameter value while repeating the operations in steps 2-4.

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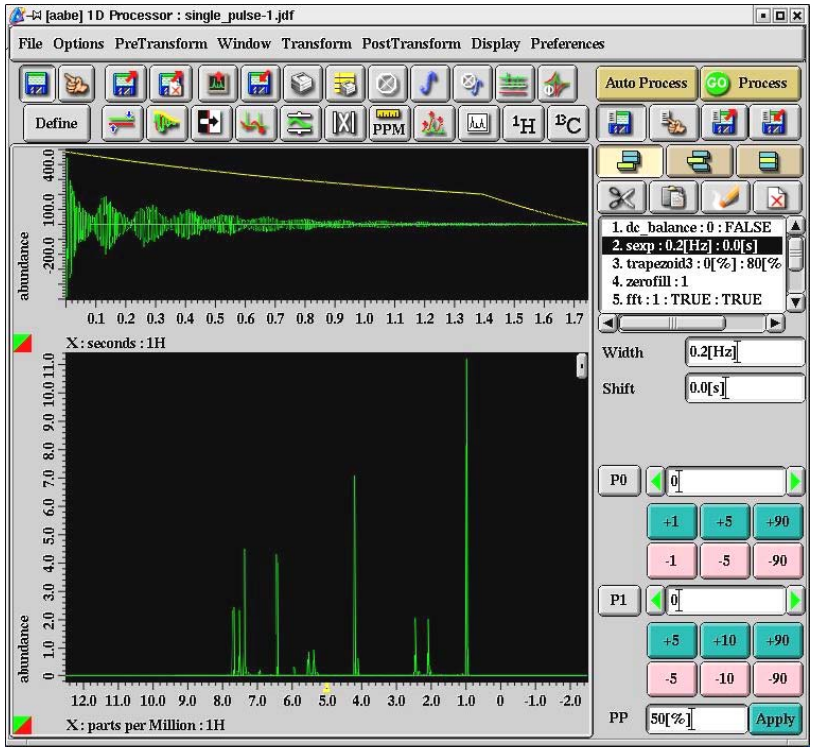
2.2.3c To Change the window function:

1. Select the window function from the process list.



The window function will be highlighted.

2. Click on the **Change** button.

3. Select the target window function from the **Window** menu of the menu bar.

The window function of the process list will change to the selected window function.

4. Click on the **Process** button.

The spectrum re-processed with the changed window function will appear in the processing data display area.

Change the parameter values of the selected window function, if required.

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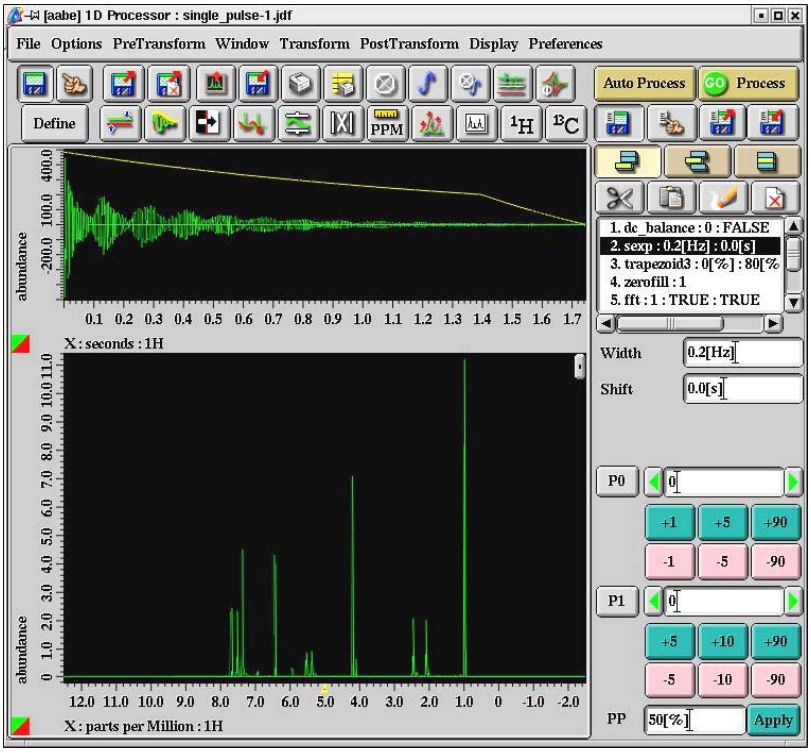
2.2.3d To Set two or more window functions:

Two or more window functions can be set up. These settings are performed separately, and their combination is calculated. The functions are combined in the input data.

1. Click on the window function in the process list.



The window function is highlighted.

2. Click on the **Insert** button.

3. Select the target window function from the **Window** menus in the menu bar.

The selected window function is added above the function selected.

4. Click on the **Process** button.

The spectrum re-processed using the changed window function appears in the processing data display area.

Change the parameter value of the selected window function if required.

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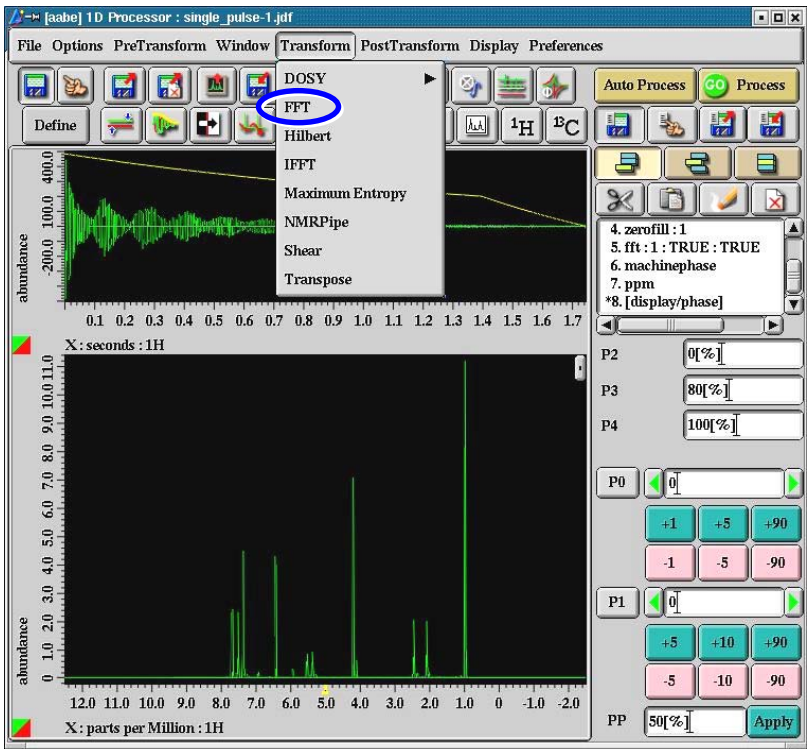
2.2.4 Fast Fourier Transformation

The time domain spectrum is changed to the frequency domain spectrum by Fast Fourier transformation (FFT).

1. Select **Transform–FFT** from the menu bar in the **1D Processor** window.



The **fft** process is added to the process list.
In FFT, one argument is attached to the process. This argument is displayed in the **Scale** input box. It corrects processing of the starting point of the FID. In the case of one-dimensional data processing, **1** is set up.

2. There are two flags in FFT, you may change them if required.

Clip performs clip processing at the time of FFT for data using the digital filter. Generally, TRUE is specified. It is ignored for data using only an audio filter.

Norm performs normalizing signal intensity. Generally speaking, TRUE is specified.

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2.2.5 Phase Correction

This corrects phase distortion of the spectrum after FFT. Both manual and automatic phase correction are provided as methods of phase correction.

2.2.5a Automatic phase correction

Two kinds of processes, **Machine Phase** and **Automatic Phase**, are provided for automatic phase correction.

Machine Phase is the function used to obtain a P1 phase from calculations based on measurement conditions. This offers the advantage of the high accuracy P1 phase correction without regard to spectrum line shape. However, **Machine Phase** supports only pulse sequences for a **Single Pulse**.

Automatic Phase is the method of obtaining phase from the spectrum line shape. Although the general pulse sequence is supported widely, the accuracy of phase correction depends on the line shape and the spectrum baseline.

◆ Select **PostTransform–Phase–Machine Phase** or **PostTransform–Phase–Automatic Phase** in the **1D Processor** window.

Automatic phase correction processing is included in the process list.

✍ If you click on the **Machine phase** button in the **1D processor** window, **Machine phase** is included in the process list.

2.2.5b Manual phase correction

Zero and first order phase correction are performed manually.

There are two kinds of correction methods: changing values in the phase parameter box, and using the cursor tool.

■ Phase correction using the phase parameter box

1. Verify that the processing of the process list is complete.

Verify that the * mark is displayed after **display/phase** processing in the process list. When the * mark is not displayed after **display/phase** processing, click on the **Process** button to complete processing.

2. Set up the phase reference position.

a. Select the **Pick** mode from the cursor tool in the processing data display area.

b. Click on the **Pick position** button in **Pick** mode.

c. Click on the peak position (the peak used for P0 correction) of maximum intensity in the processing data display area.

The pick position marker is displayed on the clicked position.

Position information for the pick position marker is displayed in **PP** in the display phase correction parameters.

✍ Usually set a pick position at the position corresponding to the biggest peak in the spectrum. However, do not select the peak at the end of the spectrum.

3. Correct the zero-order phase (P0) parameter.
   a. Select **Zoom** mode from the cursor tool in the processing data display area.
   b. Click on the **Zoom Data** button in **Zoom** mode.
   c. Expand the maximum peak whose pick position marker is displayed in the horizontal direction.
   d. Correct the phase of the peak whose pick position marker is displayed while changing its value using the **Arrow** button of the display phase correction parameter **P0.**
   e. Press the **Home** key to reset an expansion of the horizontal direction.
4. Correct the first order phase parameter (P1).
   a. Expand the suitable peak that is separated from the maximum peak whose pick position marker is displayed to the horizontal direction.
   b. Change the value using the **Arrow** button of a display phase correction parameter **P1** to correct the peak phase.
   c. Press the **Home** key to reset expansion in the horizontal direction.
5. Verify the phase.
   In the case where the phase is not correct, repeat steps 3 to 4 again.
6. Click on the **Apply** button.
   The values of **phase** processing, and the display phase calibration parameters P0, P1, and PP are added to the process list.
   The phase correction parameters are displayed under the process list.
   The value of the display phase correction parameters **P0** and **P1** are set to **0**.
   In this stage, actual phase correction is not performed only by the phase correction value being added to the process list. Only the spectrum whose phase correction was carried out is displayed.
7. Click on the **Process** button.
   All processing items of the process list are performed, and storage of the phase information is carried out.

■ Phase correction using the cursor tool

1. Verify that the processing of the process list is complete.
   Verify that the * asterisk is displayed after **display/phase** processing in the process list. When the * asterisk is not displayed after **display/phase** processing, click on the **Process** button to complete the process.
2. Set up the reference position of the phase.
   a. Select **Phase** mode from the cursor tool in the processing data display area.
   b. Click on the **Adjust the Phase PP value** button in **Phase** mode.
   c. Click on the peak position (peak used for P0 correction) of maximum intensity in the processing data display area.

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3. Correct the zero-order phase parameter (P0).
   a. Click on the **Adjust the Phase P0 value** button in **Phase** mode of the cursor tool in the processing data display area.
   b. Adjust the phase in the peak position of maximum intensity by moving the cursor to the right and left while holding down the left mouse button after moving the cursor to the processing data display area.
4. Correct the first order phase parameter (P1).
   a. Click on the **Adjust the Phase P1 value** button in the **Phase** mode of the cursor tool in the processing data display area.
   b. Adjust the phase by moving the cursor to the right and left while holding down the left mouse button after moving the cursor in the processing data display area.
5. Verify the phase.
   In the case where the phase is not correct, repeat steps 3 to 4 again.
6. Click on the **Apply** button.
   The values of **phase** processing, and the display phase calibration parameter P0, P1, and PP are added to the process list.
7. Click on the **Process** button.
   All processing items of the process list are performed, and storage of the phase information is performed.

When two or more phase processes are set in the process list

When two or more **phase** processes are set to the process list, phase correction has the same result as it that the phase correction were carried out adding the value of **P0** and **P1**, respectively.

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2.2.6 Baseline Correction

When the baseline of an NMR spectrum corrected phase is distorted, it can be corrected by the following procedure.
Both automatic and manual baseline correction are provided.

2.2.6a Automatic baseline correction

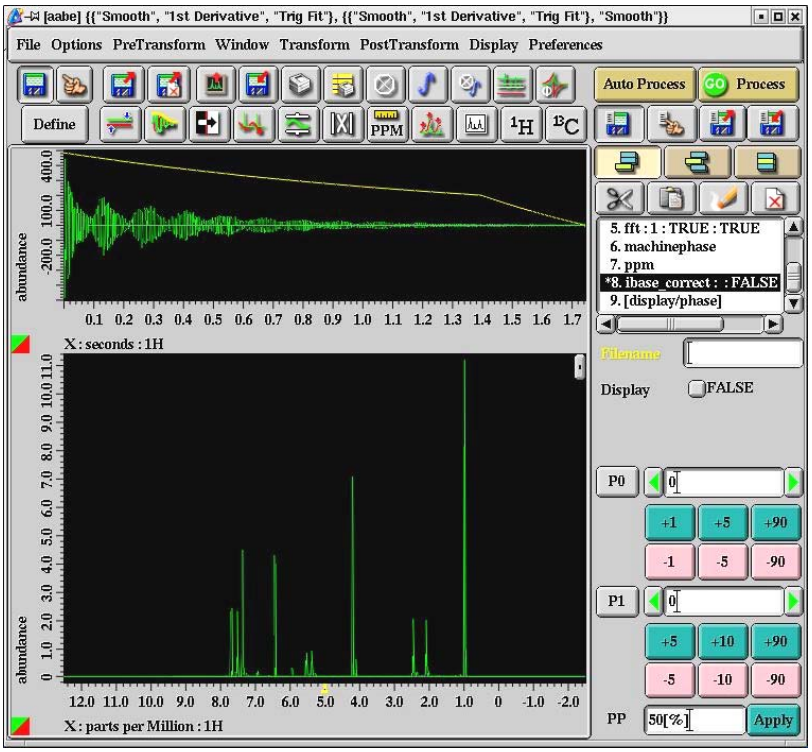
- Select **PostTransform–Baseline Correction–Baseline Correct** or click on the Base Correct button in the **1D Processor** window.

  Baseline correction processing is included in the process list.
  Execution of a process corrects a baseline.

2.2.6b Manual baseline correction

1. Select **PostTransform–Baseline Correction–Baseline Correct (Interactive)** in the **1D Processor** window.

   Baseline correction processing is added to the process list.



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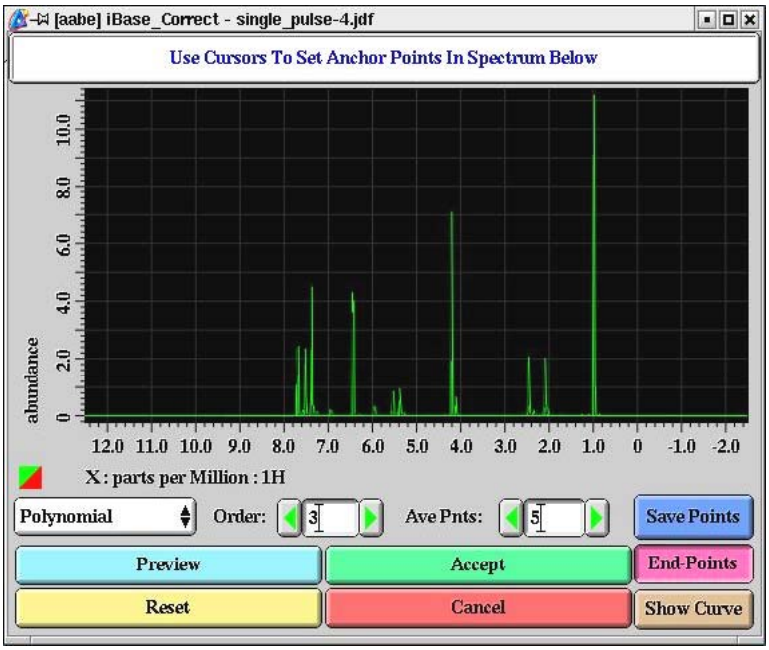
2. Click on the **Process** button.
The **IBase_Correct** window opens.



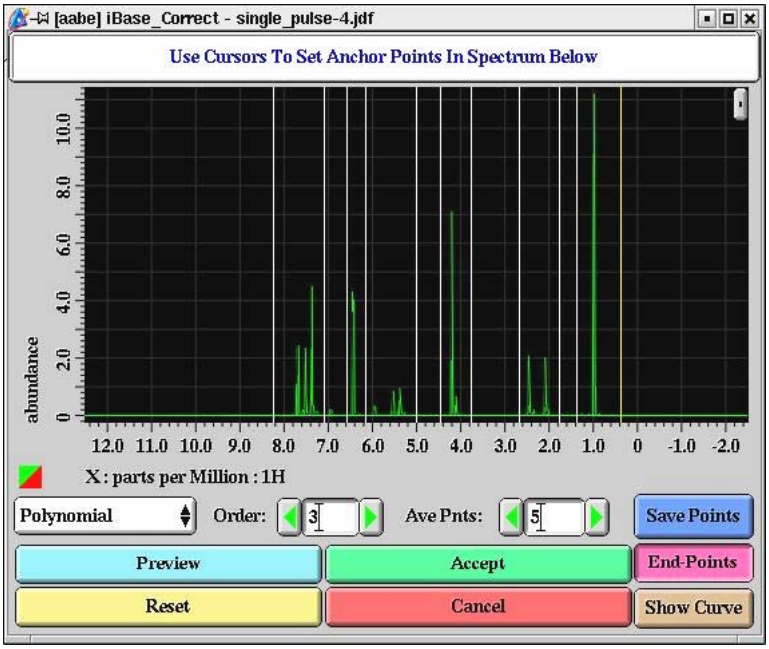
3. Select the baseline correction method.
There are the following four kinds of the correction methods.

Correction method	Explanation
Polynomial	Baseline distortion is approximated by polynomial equation.
Piecewise Linear	Baseline distortion is approximated by line graph.
Trigonometric	Baseline distortion is approximated by trigonometric function.
Akima	Baseline distortion is approximated by the Akima method.

4. Set values for the parameters **Order** and **Ave Pnts** which are used in the correction method selected in step 3.

5. Click on the **Create cursor** button in the **Cursor** mode of the cursor tool.

6. Move the mouse pointer to the processing data display area in the **IBase_Correct** window, and click a number of portions without a signal.
The base point marker will displayed.



7. Click on the **Preview** button.

The spectrum corrected baseline appears.

Furthermore, when adding or deleting a base point is required, click on the **Return to Original** button, and perform in the original spectrum.

Base points can be specified up to 32 points at once. For 32 points or more, baseline correction is repeated any numbers of times.

In the spectrum with a low signal-to-noise ratio, the specified position on a base point may be changed by a noise. At that time, the number (it centered on the base point) of averaging points for calculating the intensity of a base point is specified in the **Ave Pnts**: input box. For example, if 20 is set in the **Ave Pnts:** input box, every 10 points to the right and left of the specified base point will be calculated as the average value. The result will be used as a position of a base point.

If the **End-Points** button is turn ON, the point of both ends of the spectrum will be automatically contained in the base point.

8. Click on the **Accept** button.

Baseline correction is performed.

The **IBase_Correct** window closes, and the spectrum corrected baseline is displayed on the processing data display area of the **1D Processor** window.

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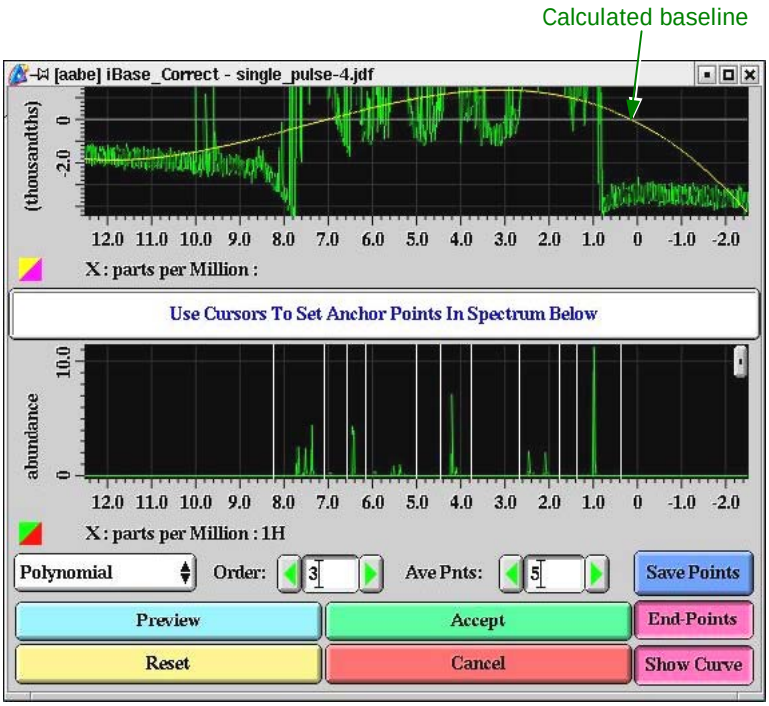
Other function in the IBase-Correct window

Check the calculated baseline

◆ Click on the **Show Curve** button.

The processing data display area is divided into two blocks. The calculated baseline is displayed in the upper row.

Click on the **Show Curve** button again to return to the original display.



To Delete the arbitrary base points

1. Click on the **Delete cursor** button in the **Cursor** mode of the cursor tool
2. Move the mouse pointer to the base point marker you want to delete, and click.

   The base point marker is deleted.

To Delete all base points

◆ Click on the **Reset** button.

All base point markers are deleted.

To Move a base point

1. Click on the **Move cursor** button in **Cursor** mode of the cursor tool.
2. Move the mouse pointer to the marker of the base point to move; press and hold down the mouse button.
3. Drag a base point marker to a position to which move you want to it.

   The base point marker moves.

2.2.7 Axis Units

The axis of the NMR spectrum can be displayed in various units. In immediately after FFT, unit is Hertz. It can be changed to ppm (parts per million) by using either of the following methods:

To use the PPM button:

- Click on the PPM button.

  The **PPM** command is inserted in the process list.

To use the Display Units command:

- Select **Display Units-ppm** in the right mouse button menu.

When you insert a **PPM** command in the process list using the PPM button, the basic axis unit in the data file is changed. When using the **Display Units** command, the axis unit is only changed temporarily in the display. Therefore, in the case of the **Display Units** command, when the data file is opened next, it returns to the original basic unit.

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2.2.8 Setting a Reference

In order to obtain an exact chemical-shift value, it is necessary to perform reference setting of the NMR spectrum

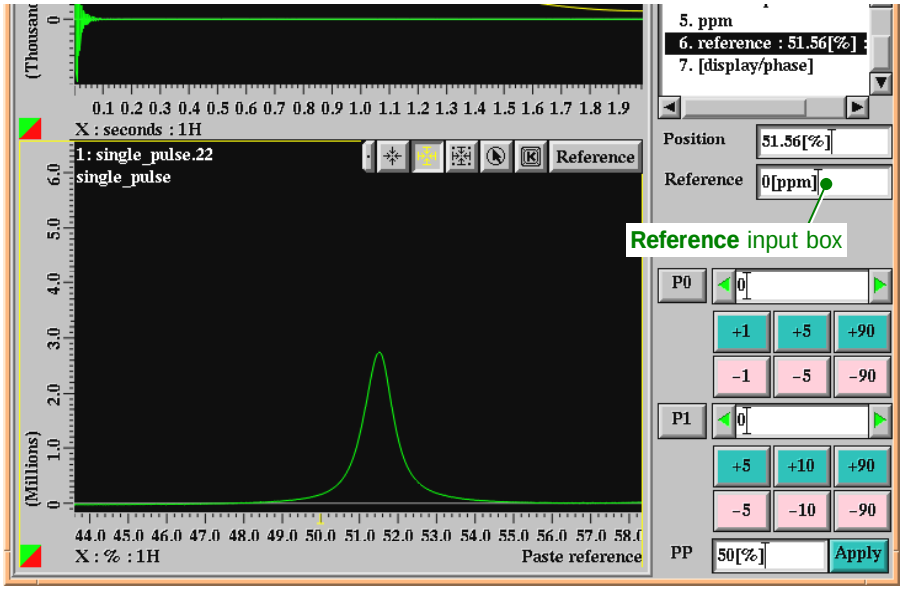
In the Delta program, the Native scale that determines the reference position from the gamma ratio and the magnetic field strength is adopted as a standard.
It is also possible to set up the reference position correctly on the basis of the reference peak, such as TMS.

To perform reference setting, there are the following three methods:

- Using the **Reference** mode of the cursor tool.
- Using the reference tool.
- Using the **Reference** command.

2.2.8a To set the reference using the cursor tool:

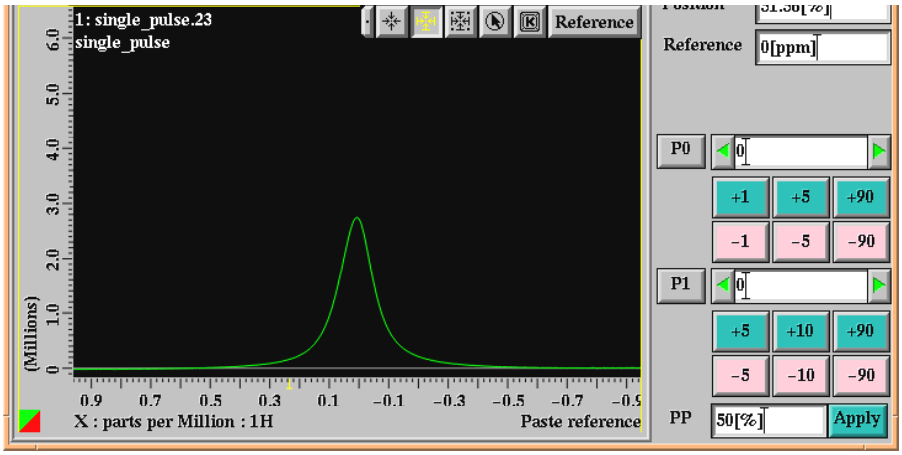
1. Select the **Reference** mode from the cursor tool in the processing data display area.
2. Click on the **Grab position for reference** button in **Reference** mode.
3. Click a position to make a reference.
4. Expand the peak made by the reference - e.g. the TMS of a reference substance, or a solvent in the direction of the X-axis.
5. Click on the **Paste reference** button in **Reference** mode.
6. Move the mouse pointer to the top of the peak to be made the reference.
7. Click on the left mouse button.
   Reference processing, **Position** of the clicked position, and the value of the **Reference** set up in step 3 is added to the process list.
   Moreover, the **Position** input box and the **Reference** input box appear under the process list.
8. Input the reference value into the **Reference** input box from the keyboard if required.
   The **Reference** value of the process list changes to the entered value.
   ✍ Enter with ppm unit.



9. Click on the **Process** button.

Processing of the process list is performed.

The position of **Position** becomes the **Reference** value.



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2.2.8b To Set the reference using the reference tool:

1. Select **Analysis**–**Reference** in the **Delta Console** window, or select **options**–**Reference** in the **1D Processor** window.
   The reference tool starts, then the **Enter Reference Values** window opens.

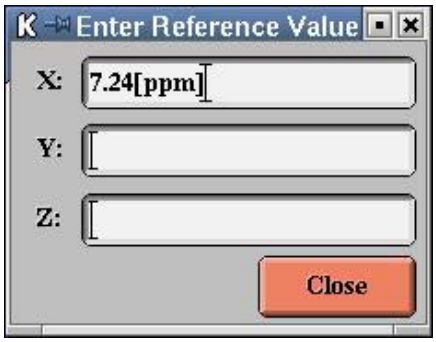

Fig. 2.2 Enter Reference Values window

2. Enter the reference value of the X-axis into the **X** input box.
3. Select the **Paste reference** button in the **Reference** mode of the cursor tool, and click on the position that performs the reference setting in the spectrum.
   A new reference value is set in the clicked position, and the axis is changed.

In the **Reference** mode of the cursor tool, the value of the reference can be read from the data se. The reference value can also be zero.

Button name	Function
Paste reference	Pasts a reference value to the spectrum.
Grab position for reference	Copies a reference value from the spectrum, and displays the value on the numerical box of the **Enter Reference Values** window.
Key command display	This is used when making the reference value to zero.

2.2.8c To set the reference using the Reference command:

If you select **Display–Reference** in the **1D Processor** window, you can set a reference in an arbitrary positions. Two values of the position that sets up a reference, and a new reference value are required in the **Reference** function. These values are entered into the box displayed under the process list. Click on the **Process** button executing the process list.

References

- Copy of a reference value
  If **Analysis–Ext.Reference** is selected chosen in the **Delta Console** window, the **Copy Reference Tool** window opens. If this window is used, the reference value of the axis can be copied and pasted on top of the data of another view from one data between two data display windows (it copies). The copy the data to is called **Source**. The data of place to copy is called the **Target**.

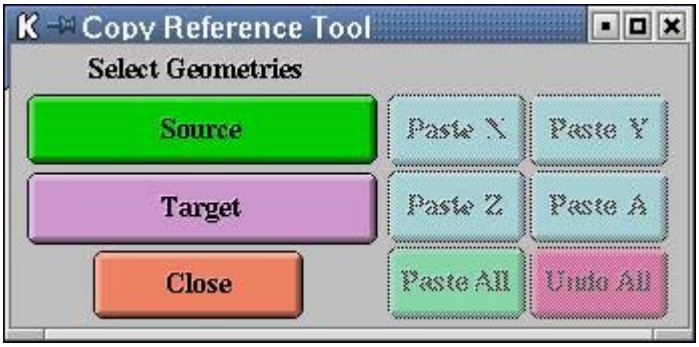

Fig. 2.3 Copy Reference Tool window

- **Maximum Reference** command
  This is used when setting the top of the signal as the reference. For example, if 0 ppm is entered in **Ref** and 0.2 ppm is entered in **Width, t6he** new 0 ppm will be set to the maximum signal in the range of 0.2 ppm centering on the present 0 ppm.
- **Auto Reference** command
  If **Display–Reference–Auto Reference** is performed in the **1D Processor** window when an NMR data is sent from the spectrometer of JEOL GSX, and EX, Alpha or Lambda, the macro program will calculate 0 ppm reference, and will apply to the data.
- For data other than JEOL, select **Display–Reference** in the **1D Processor** window, or select **Analysis–Reference** in the **Delta Console** window.
- For NMR data measured by this spectrometer, the reference is set up automatically based on the absolute frequency of the **gamma.def** and **solvent.def** files. When you change this reference setting, select **Display–Reference** in the **1D Processor** window, or select **Analysis–References** in the **Delta Console** window.

When you read an exact frequency position in the spectrum to perform a homo-spin decoupling experiment, use the spectrum before changing a reference automatically or manually (in the state in which the instrument is set up initially).

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2.2.9 Peak Detection

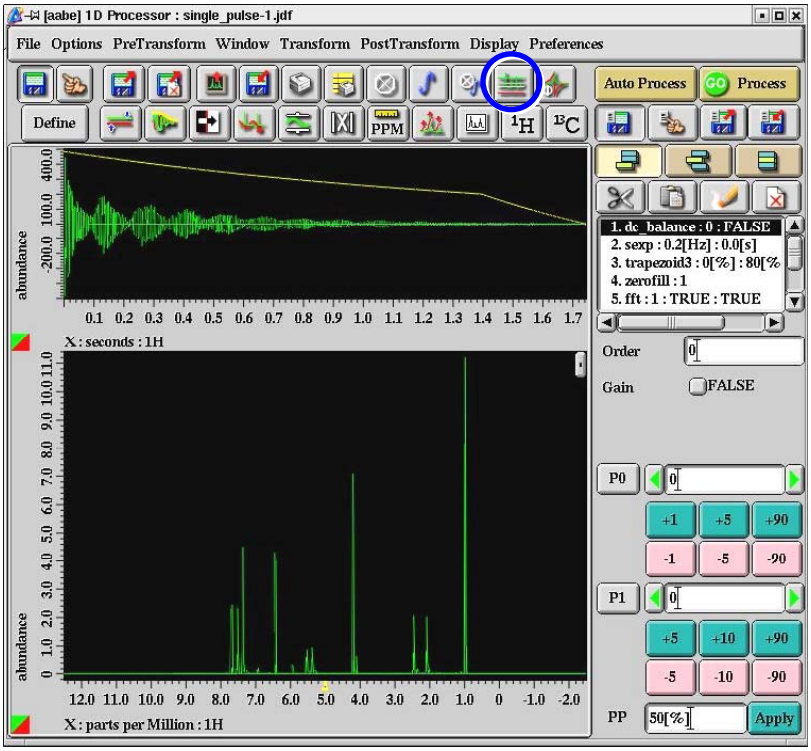
For the peak detection method of a spectrum, both automatic and manual detection are provided.

2.2.9a Automatic peak detection

◆ Click on the **Auto Peak Pick** button.
In this case, both the threshold and noise level are calculated automatically.

Moreover, the base level, noise level, and threshold level are set up, and automatic peak pick can also be performed.

1. Click on the **Compute and Show Statistics** button.



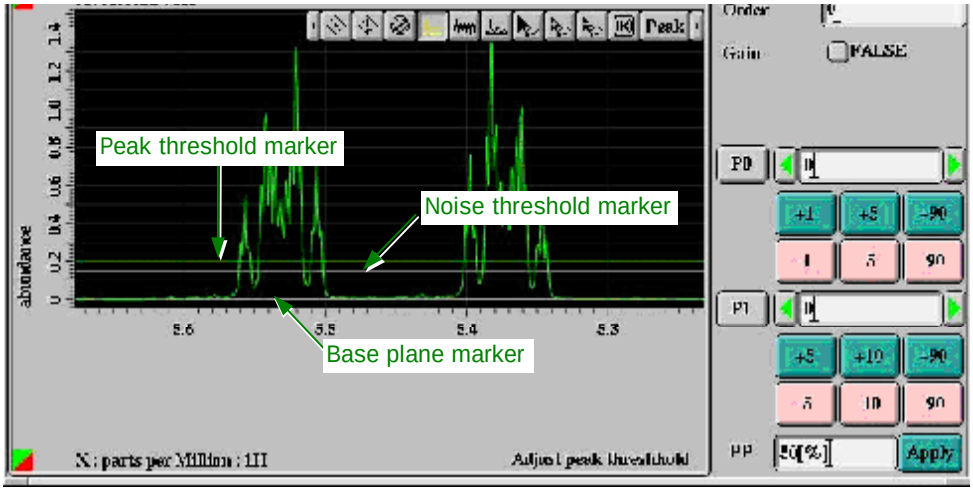
The markers of the peak threshold level, noise threshold level, and base plain level are displayed on the processing data display area.
Each level marker at this time is displayed in a position calculated automatically.

2. To set up the peak threshold level in the following procedure.

a. Click on the **Adjust peak threshold** button in the **Peak** mode of the cursor tool.

b. Move the mouse pointer to the processing data display area; press and hold down the mouse.
The peak threshold level marker moves to the position where the mouse was clicked.

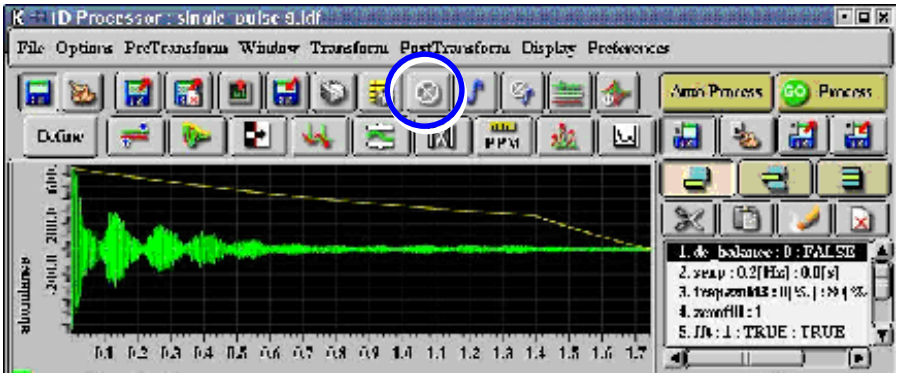
c. Move the mouse pointer to a suitable position while holding down the mouse button, and release the mouse button.
The peak threshold level marker moves to the position that released the mouse.



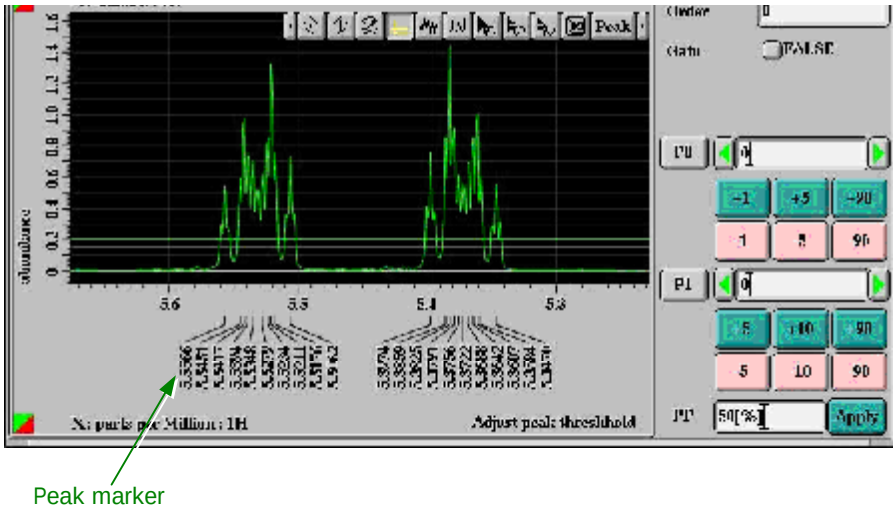
3. To set up the noise threshold level:
   a. Click on the **Adjust noise threshold** button in **Peak** mode of the cursor tool.
   b. Move the mouse pointer to the processing data display area; press and hold down the mouse button.
      The noise threshold level marker moves to the position at which the mouse was pressed.
   c. Move the mouse pointer to a suitable position while holding down the mouse button, and release the mouse button.
      The noise threshold level marker moves to the position at which the mouse was released.

4. To set up the base plain level:
   a. Click on the **Adjust base plane/threshold** button in **Peak** mode of the cursor tool.
   b. Move the mouse pointer to the processing data display area; press and hold down the mouse button.
      The base plain level marker moves to the position at which the mouse was pressed.
   c. Move the mouse pointer to the baseline of the spectrum while holding down the mouse button, and release the mouse button.
      The base plain level marker moves to the position at which the mouse was released.
      In connection with moving a base plain level marker, the peak and noise threshold level marker also move.

5. Click on the **Auto Peak Pick Spectrum** button.



Peak detection is performed and the peak markers are displayed.



Reference

If you click on the **Peak Pick & Integrate** button in the **1D Processor** window, automatic peak detection and automatic integration will be performed, and the result will be displayed on the processing data display area in the **1D Processor** window.

2.2.9b Manual peak detection

It is necessary to set up the threshold value and noise level value described above. Moreover, this method is also a method for adding or deleting a detection peak after automatic peak pick.

■ To add a peak specifying a suitable position:

1. Click on the **Create peak** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer near the top of the peak to add, and click on the mouse button.
   The peak of the clicked position is detected automatically, and the peak marker is displayed.

If you want to specify or add the peak exceeding threshold and noise level set up now using the **Create peak** button, a warning message **No Peak exceeds threshold** will be displayed. The peak below threshold set up cannot be specified or added.

■ To add a specified position as a peak:

1. Click on the **Force create peak** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer to the position added as a peak, and click on the mouse button.
   The clicked position is detected as a peak, and a peak marker is displayed.

■ To delete arbitrary detection peaks:

1. Click on the **Delete peak** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer to the position which overlaps with the peak marker of the peak to delete, and click on the mouse button.
   The clicked peak marker is deleted.

■ To delete a selected peak

1. Select the peak to delete.
   Select a peak according to the "■Select only one peak marker" described next.
2. Press the **Cursor tool** button (key command display button), and click on **Delete [Del]** in the pull-down menu displayed.
   The selected peak marker is deleted.

■ Selecting only one peak marker

1. Click on the **Select peaks** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer to the position which overlaps with the peak marker of the peak to select, and click on the mouse button.
   The clicked peak is selected. The selected peak changes the color of a peak marker, and the # mark is displayed on the peak.

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To select all the peaks within a certain range

1. Click on the **Select peaks** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer to the left of the peak marker group in the range to select; press and hold down the mouse button.
   Vertical cursor appears.
3. Move to the right of the peak marker group in the range to select while holding down the mouse button, and release the mouse button.
   All the peaks in the range enclosed with the vertical cursor are selected. The selected peaks change the color of the peak markers, and "#"s are displayed on the peaks.

To Select all the peaks

- Press the button in the cursor tool, and click on **Select All [A]** in the pull-down menu displayed.
  All peaks are selected. The selected peaks change the color of the peak markers, and "#"s are displayed on the peaks.

To choose two or more peaks in the separated position

1. Click on the **Select more peaks** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer to the position which overlaps with the peak marker of the peak to select, and click on the mouse button.
   The clicked peak is selected. The selected peaks change the color of the peak markers, and "#"s are displayed on the peaks.
3. Furthermore, move the mouse pointer to the position which overlaps with the peak marker of another peak to select, and click on the mouse button.
   The clicked peaks are selected. The selected peaks change the color of the peak markers, and the # marks are displayed on the peaks.

To cancel a certain peak selection

1. Click on the **Unselect peaks** button in **Peak** mode of the cursor tool.
2. Move the mouse pointer to the position which overlaps with the peak marker of the peak to cancel, and click the mouse button.
   Selection of the clicked peak is canceled.

Canceling all the peaks selection in a certain range

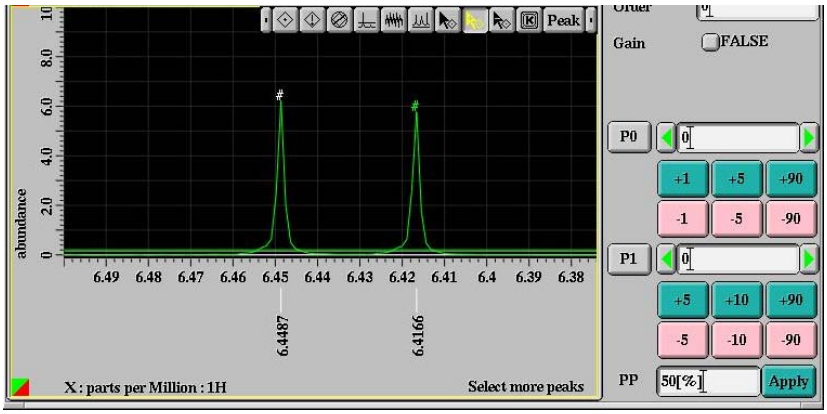
1. Click on the **Unselect peaks** button in the **Peak** mode of the cursor tool.
2. Move the mouse pointer to the left of the peak marker group in the range released selection; press and hold down the mouse button.
   The vertical cursor appears.
3. Move the mouse pointer to the right of the peak marker group in the range canceled selection while holding down the mouse button, and release the mouse button.
   Selection of all the peaks in the range enclosed with the vertical cursor is canceled.

To display the J value between peaks:

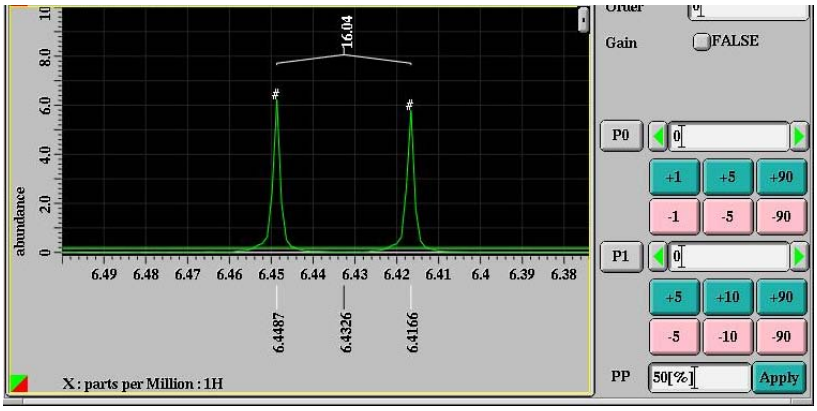
1. Click on the **Select more peaks** button in the **Peak** mode of the cursor tool.

2. Move the mouse pointer to the position that overlaps with the peak marker of the peak you want to select, and click on the mouse button.
   The clicked peak is selected. The selected peak changes the color of a peak marker, and "#" is displayed on the peak.

3. Then, move the mouse pointer to the position that overlaps with the peak marker of another peak, and click on the mouse button to select it.
   The clicked peak is selected. The selected peak changes the color of a peak marker, and "#" is displayed on the peak.



4. Press the button (key command display button) in the cursor tool, and click on **J Coupling [J]** in the pull down menu displayed.
   The J value between the selected peaks is displayed.



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For changing the unit of a peak marker label

1. Select **Display Units**–**Peak Units** from the right mouse button menu.
2. Select a unit from menus.

   Hertz
   ppm
   Percent
   Point
   Ruler Units

   The label of the peak marker changes to the selected unit.

The display format of a peak list

In the default, a peak list is displayed under a spectrum. If you select **Options –Peak–Peak Above** from the mouse right button menu, a peak list can be displayed on a peak.

2.2.10 Integration

Manual and automatic integration are provided for the spectrum.

2.2.10a Automatic integration

The automatic integration algorithm uses the threshold and noise value.
Usually, these values are calculated automatically.

- Click on the **Auto Integration** button after setting threshold and noise levels.
  Integration is performed.

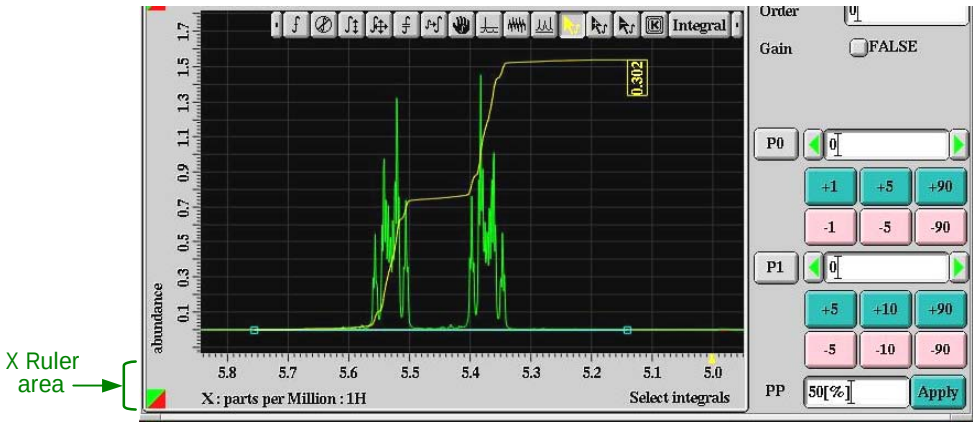
Reference: If you click on the **Peak Pick and Integrate** button in the **1D Processor** window, automatic peak detection and integration will be performed. The result will be displayed on the processing data display area in the **1D Processor** window.

2.2.10b Manual integration

This method is also the same as the method for adding or deleting integration after automatic integration.

■ To add the integration curve

1. Select **Integral** mode from the additional cursor tool in the data processing display area.
2. Click on the **Create integral** button.
3. Move the pointer to the **X Ruler** area at the left of the integration range where you want to add an integration curve; press and hold down the mouse button.
   The vertical cursor appears.

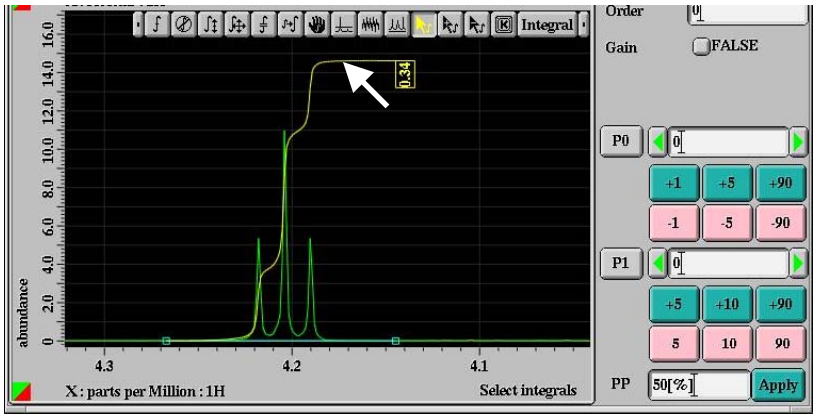


4. Move the cursor to the right of the integration range in the **X Ruler** area while holding down the mouse button, and release the mouse button.
   An integration curve is added.
5. Repeat the operation of steps 3-4 to add the required integration.

Reference: The difference of the base point level according to the specified different integration range.
When the integration range is specified in the **X Ruler** area by the method described above, the level of an integration base point is set to the point strength position of a spectrum.
When the integration range is specified within the processing data display area, the integration base point level is set the position of the starting and stopping points which are specified using the mouse.

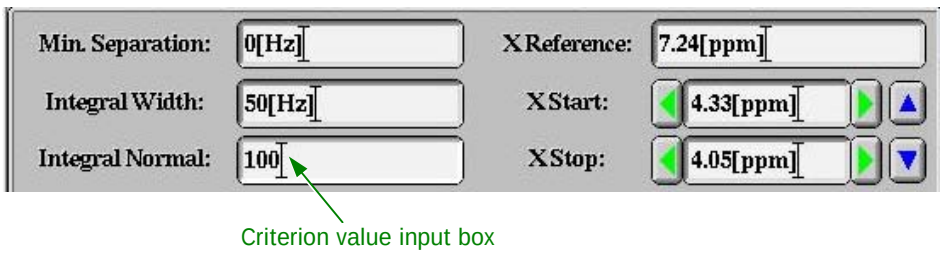
■ To set the current integration

1. Click on the **Select integrals** button in the **Integral** mode of the cursor tool.
2. Move the mouse pointer onto the integration curve set to current integration, and click the mouse.
   The color of the selected integration changes to yellow.



■ To set an integral criterion value

1. Set the integration whose criterion value you want to specify to the current integration referring to "■ setting current integration".
2. Press the button in the cursor tool; then click on **Normalize [N]** in the pull-down menu displayed.
   The integration value of the integration selected in step 1 is set to the criterion value, and the other integration values also change relatively according to the criterion value. When you have changed the criterion value, perform steps 3 and 4.
3. Select **Options–Show Options** from the menu bar.
   Place a check mark to **Options–Show Options** in the **1D Processor**. The following input box appears in the FID display area.



4. Set a criterion value for the criterion value input box using the key board.
   The integration value changes.

To delete arbitrary integration curves

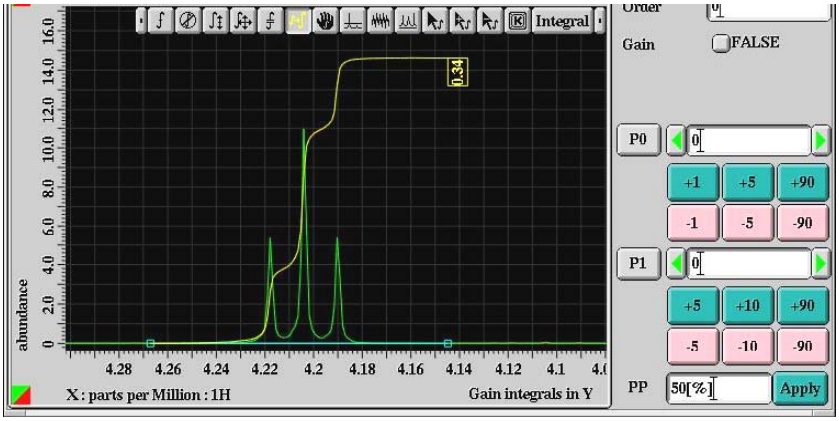
1. Click on the **Delete integrals** button in the **Integral** mode of the cursor tool.
2. Move the mouse pointer onto the integration curve you want to delete, then click on the mouse.
   The selected integration is deleted.

To Delete all integration curves:

1. Press the button in the cursor tool, and click on **Select All [A]** in the pull-down menu that is displayed.
   All integration changes to the color of the selection state.
2. Press the button again, and click on **Delete [Del]** in the pull-down menu that is displayed.
   All of the integration curves are deleted.

To change the size of an integration curve:

1. Click on the **Gain integral in Y** button in the **Integral** mode of the cursor tool.
2. Move the mouse pointer to the processing data display area.



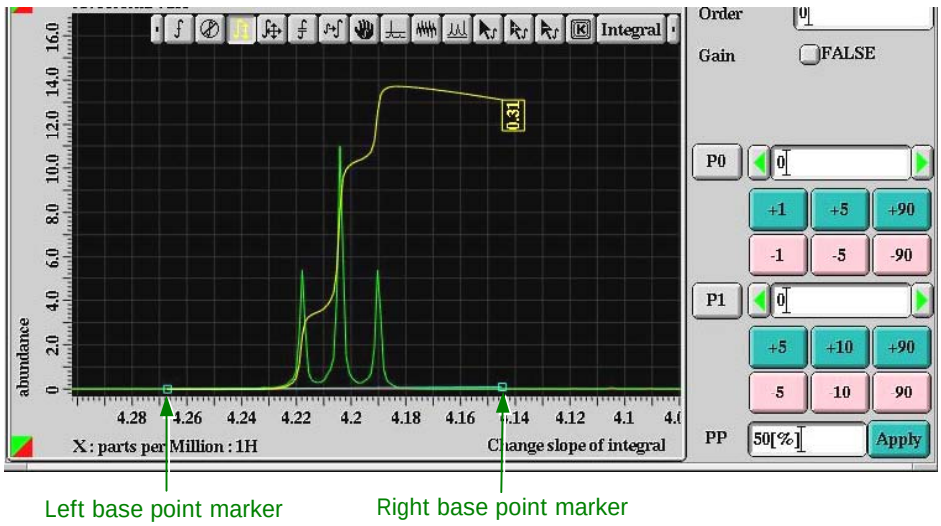
3. Press and hold down the mouse button.
4. Move the mouse pointer to change the size of an integration curve, and release the mouse button.
   Expansion will be performed if the mouse pointer is moved upward, and reduction will be performed if the mouse pointer is moved downward.

■ To change the display position of an integration curve:

1. Click on the **Change integrals offset** button in the **Integral** mode of the cursor too.
2. Move the mouse pointer to the processing data display area.
3. Press and hold down the mouse button.
   The horizontal cursor appears.
4. Move the level cursor to a suitable position, and release the mouse button.
   The left end of the baseline of the integration curve moves to the position of the cursor.

■ To correct an integral baseline

1. Set the integration whose integration baseline you want to correct to the current integration referring to "■ Setting current integration" described above.
   An integration baseline and base point markers appear.
2. Click on the **Change integral slope** button in **Integral** mode of the cursor tool.
3. Move the mouse pointer near the base point marker to the right or left.



4. Click on the mouse button at a suitable position.
   The base point moves to the position selected, and the baseline of the integration curve changes.
5. Repeat steps 3 and 4 while verifying the integration curve.

2.2.11 Transfer Integral Tool Window

If you use the **Transfer Integral Tool** window, creation, saving and reading of integration conditions can be performed. The created integration conditions (it is called an integration template) can be directly applied also to the data of another window. An integration template is a list of integration ranges. You must specify N to the integration to be made the criterion.

1. Select **Analysis–Transfer Integral Tool** from the menu bar in the **Delta Console** window.

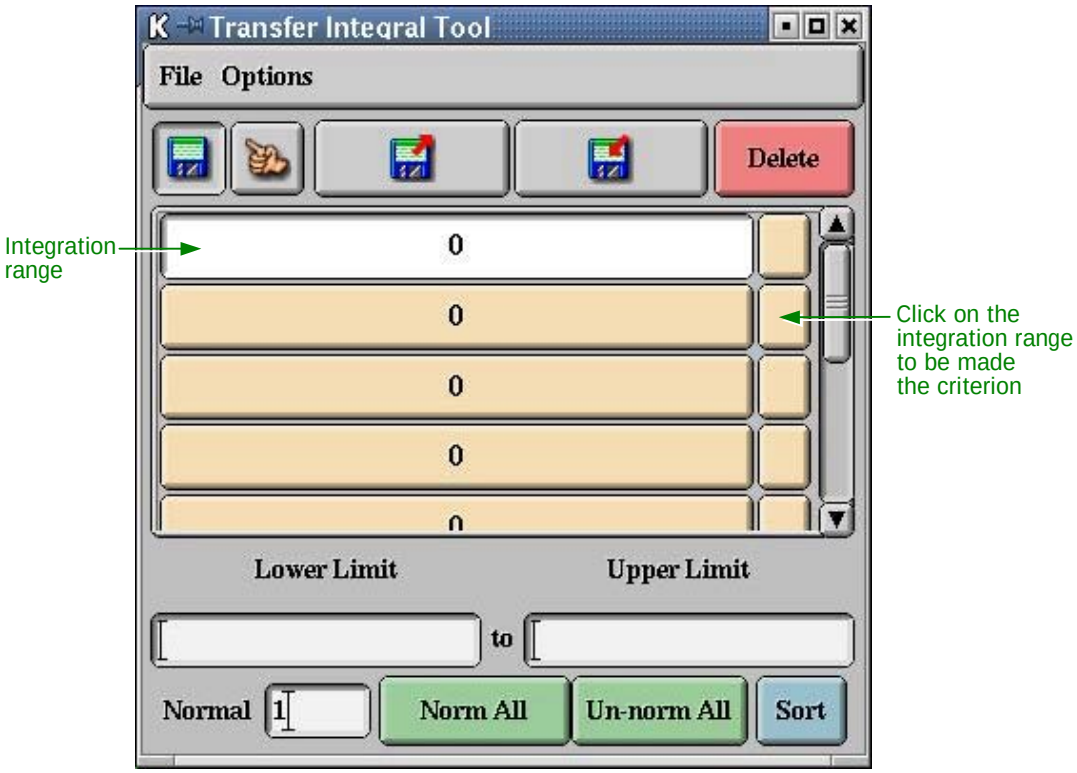


Fig. 2.4 Transfer Integral Tool window

2. Click on the Set Source of Integral Information to a Geometry button.

3. Click on the Apply Integral Information button.
The mouse pointer changes to a finger.

4. Click on the spectrum to refer.
The integration range is referred, and integration is performed.

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2.2.12 Comment

You can write a comment (character) on the screen in Delta. The comment is created in the **Annotation** mode of the cursor tool.
When displaying a comment, select **Options–Annotations** in the right mouse button. The comment is saved together with data. Save the data set at a hard disk after creating a comment.

■ To create a comment

1. Select **Annotation** mode from the cursor tool.
2. Select the **Create text annotation** button in **Annotation** mode.
3. Move the mouse pointer to the position where it creates a comment, and click on the left mouse button.
   The mouse pointer changes to a text cursor [|]. At this time, the input direction can be changed using the Page Up or Page Down key.
4. Type a text from the keyboard.
   A Greek character can be input if you type it while pressing the Alt key. In addition, any one line comment can be entered.
5. Press the Enter key.
   Comment input finishes.

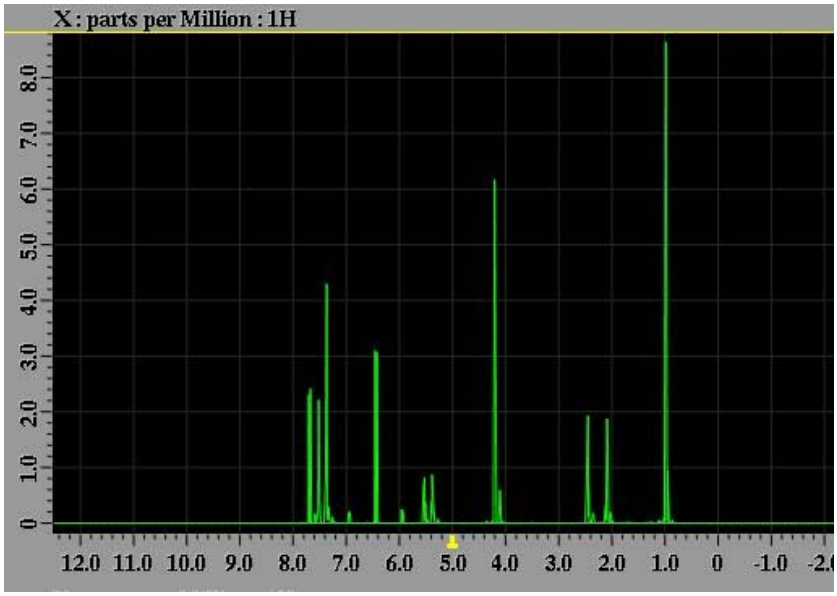

Fig. 2.5 Data before writing in a comment

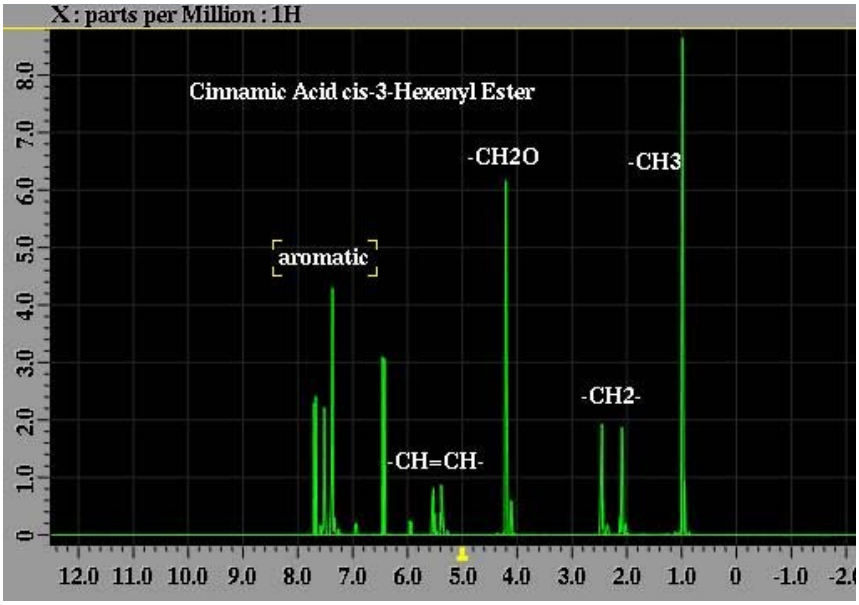

Fig. 2.6 Data after writing in a comment

To edit a comment:

1. Select the **Annotation** mode from the cursor tool.
2. Click on the **Edit text annotation** button in **Annotation** mode.

3. Select the comment to edit using the left mouse button.
   Click on near the lower left of the comment to edit it.
   The selected comment is surrounded by a yellow frame.
4. Move the | marker position using the <- or -> key on the keyboard, and edit the character line.
5. Press the Enter key.
   The edit finishes.

To move a comment:

1. Select the **Annotation** mode from the cursor tool.
2. Click on the **Move/Resize annotation** button in the **Annotation** mode.
3. Select the comment that you want to move.
   The selected comment is surrounded by the yellow frame.
4. Move the mouse pointer to the position of a transfer place, and release the mouse button.

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To change the font and size of a comment:

1. Select **Annotation** mode from the cursor tool.
2. Click on the **Select annotation** button in the **Annotation** mode.
3. Select the comment to change using the left mouse button.
   The selected comment will surrounded by the yellow frame.
4. Click on the right mouse button.

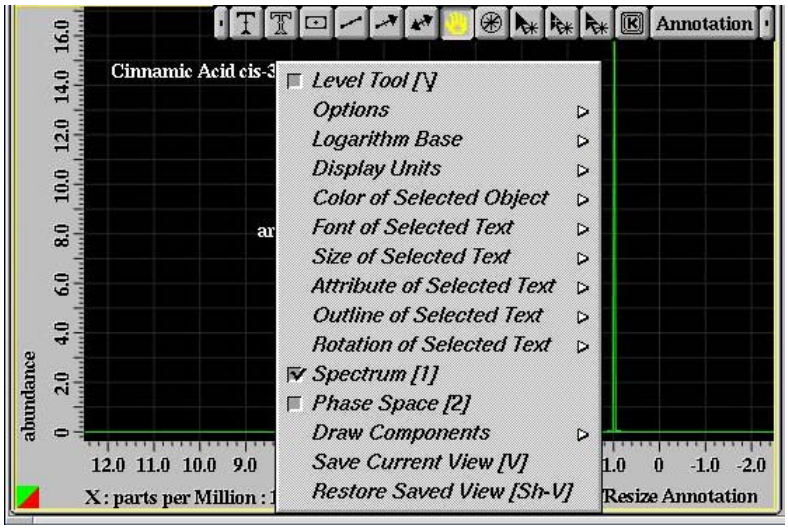

Fig. 2.7 Pressing the right mouse button.

The change will be displayed.

5. Move the cursor to select a new font.

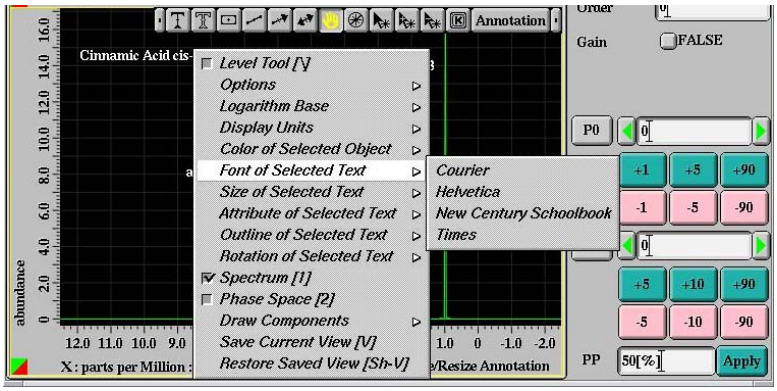

Fig. 2.8 Font of Selected Text is selected.

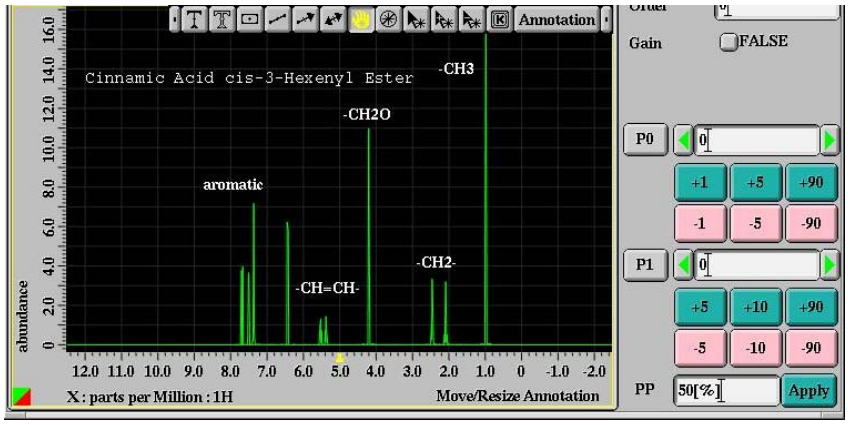

Fig. 2.9 The font is changed

The font will be changed.
In addition, select other comments to perform changes as in color to shown below.

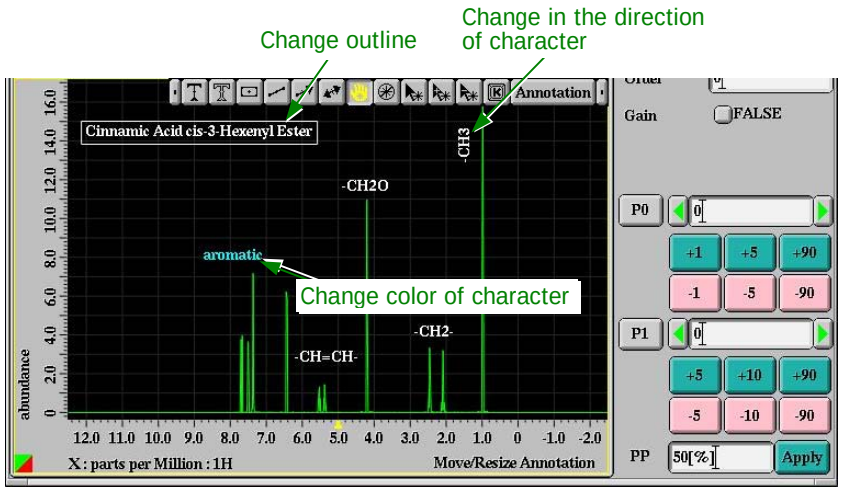

Fig. 2.10 Changing a comment's color

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2.2.13 PIP (Picture In Picture)

PIP is the function which creates a partial spectrum (child geometry) from the whole spectrum (parent geometry). This function is used when viewing a part of the spectrum in detail. This is done using the **PIP** mode of the cursor tool.

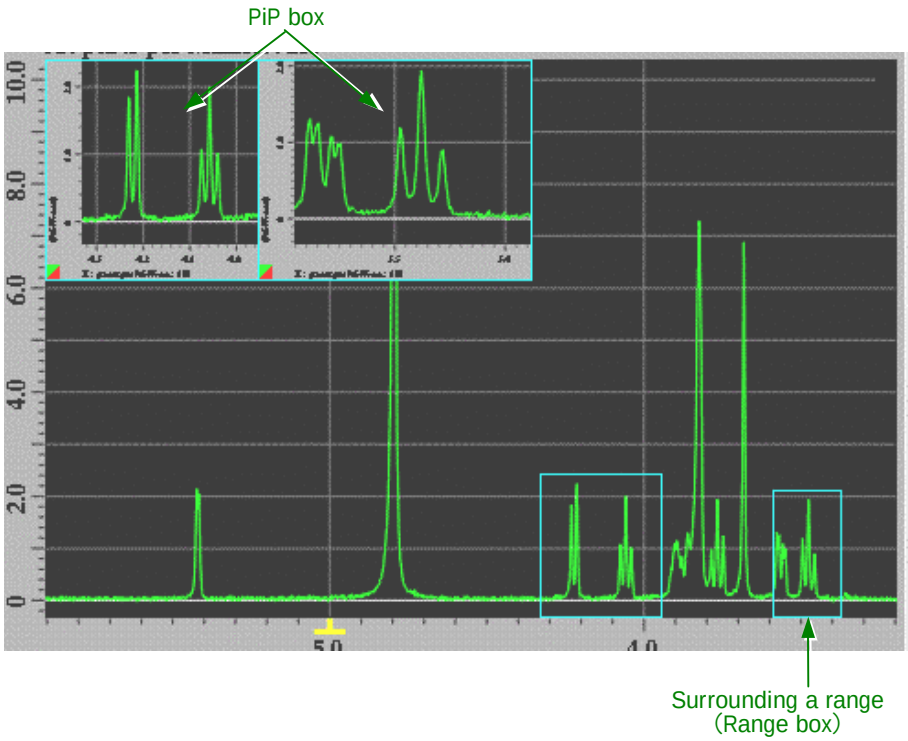


Fig. 2.11 Data-processing display area after PIP performing

■ To create a PIP box:

1. Select the **PIP** mode from the cursor tool.
2. Click on the **Create PIP by zoom region** button in the **PIP** mode.
3. Drag the left mouse button to surround the range to be made into a PIP.
   A partial spectrum (PIP box) is displayed overlapping on the enclosure (range box) where the specified range appears on the blue box.
4. Move the PIP box according to the "■To move the PIP box".

■ To move PIP box

1. Select the **PIP** mode from the cursor tool.
2. Click on the **Move/Resize PIP** button in the **PIP** mode.
3. Move the mouse pointer into the range of the PIP box, and drag it.
   The selected PIP box moves. Drag it to the position whose partial spectrum can be easily seen.

Other functions in PIP mode

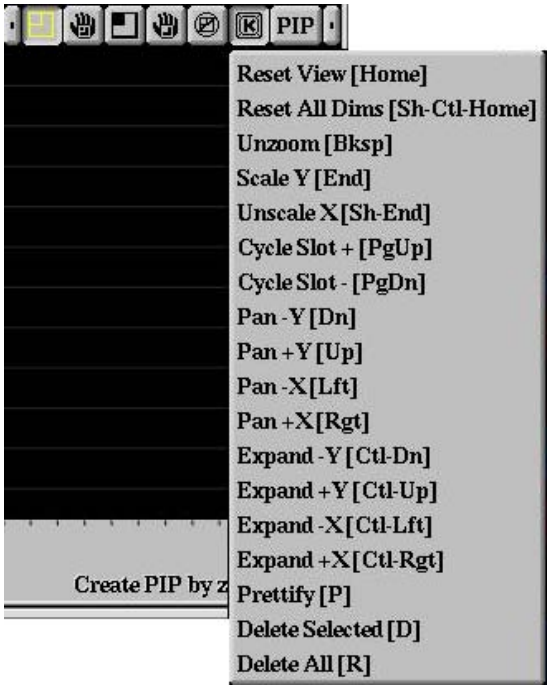
There are also the following functions in the cursor tool **PIP** mode .
The transfer and resizing of a domain box (blue) which were displayed on the whole.

Move/Resize PIP zoom region button:
Moves and resizes the range box (blue by default) displayed in the whole spectrum. The PIP box range may also be changed simultaneously.

Delete PIP button: Deletes the selected PIP box. Click on the center mouse button to the PIP box that you want to delete.

To arrange the PIP box:

- Select **Prettify** from **PIP** mode, or press the P key on the keyboard.



The PIP box aligns.

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2.2.14 To Set Up the Display Area of a Spectrum:

You can set up the display area of a spectrum numerically.

1. Move the mouse pointer to **Tools**–**Analysis**–**View Control** in the menu bar of the **Delta Console** window, and release the mouse button.
The **View Control** window opens.

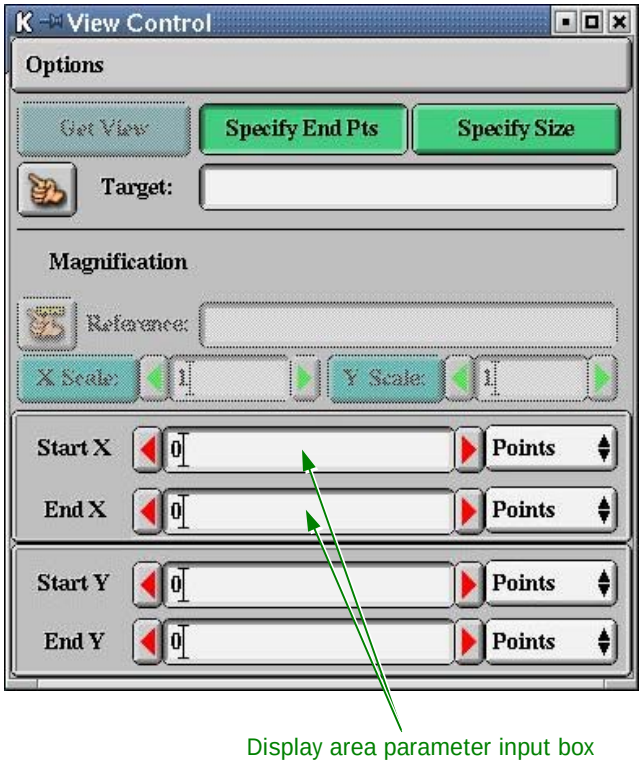


Fig. 2.12 View Tool window

2. Click on either the **Specify End Pts** or **Specify Size** button:

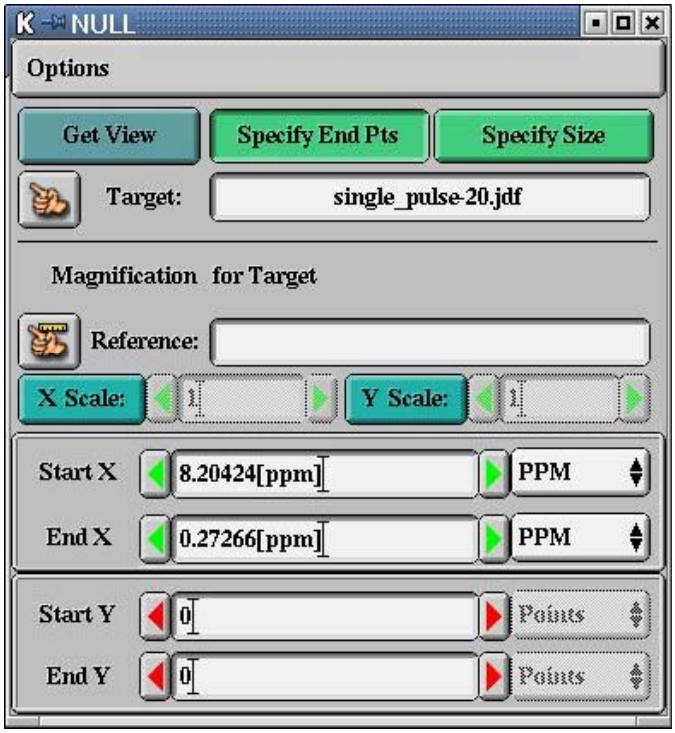
Specify End Pts: When the display area is set up using the starting point **Start X** and a stopping point **End X**.

Specify Size: When the display area is set up using the center position **Center X** and expansion width **Size X** of an expansion.

3. Click on the Open Data By Finger Geometry button.
The mouse pointer changes to the finger.

4. Move the mouse pointer to the area where the spectrum to expand is displayed, and click on the left mouse button.
The file name of the clicked data is displayed on **Target** in the **View Tool** window. Furthermore, the display area of the present is displayed on the display area parameter input box.

5. Enter the range displayed to the display area parameter input box numerically using the keyboard.
The display area of the data clicked in step 4 changes.



The value displayed on the display area parameter input box is the present display area. Since the value inputted from the keyboard is rounded by the digital resolution of the spectrum, the values actually displayed are input values.

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2.2.15 Printing

Delta supports the output in PostScript. Printing of the routine can be simply performed using the following procedures.
In addition, to customize printing conditions, use the **Presentation Manager** window.

■ Printing data

◆ Click on the **Plot Processed Data** button in the **1D Processor** window
A is clicked.

The processed data with its selected parameters are printed.
Perform parameter selection according to the following instructions "■ To select printing parameters."

■ To select printing parameters

The printing data and parameters can be selected from the following four items:

- Only processing data.
- Processing data and measurement parameters.
- Processing data, processing parameters.
- Processing data, processing parameters, and measurement parameters.

◆ Set up the printing or not printing data of a data processing by clicking on the **Preferences**–**Plot Params** toggle button in the menu bar of the **1D Processor** window, and turn ON/OFF the **Preferences**–**Plot Process List** toggle button.

- Only processing data:
  Turn OFF both **Plot Params** and **Plot Process List**.
- Processing data and measurement parameters:
  Turn ON **Plot Params,** and turn OFF **Plot Process List.**
- Processing data and processing parameter:
  Turn ON **Plot Params,** and turn OFF **Plot Process List**
- Processing data, processing parameters and measurement parameters:
  Turn ON both **Plot Params** and **Plot Process List.**

After this, click on the **Plot Processed Data** button. The processing data and the parameters selected above are printed.

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Reference

When you plot explanatory notes, such as peak comment, and sample names, measurement conditions, in arbitrary places of the processing data display area, refer to the section 2.2.12 " Comment".

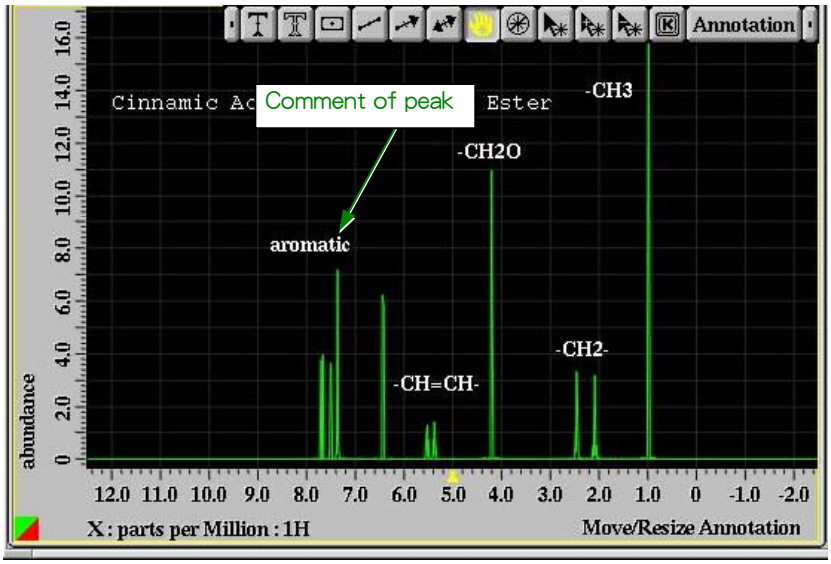

Fig. 2.13 Printing screen

Setting of a routine plot can be performed by **Preference–Plot Params**.

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2.3 Deconvolution

If you use deconvolution, overlapping NMR peaks can be separated. Separation can be performed by optimizing a waveform parameter by approximating the observation spectrum with which two or more peaks overlapped by superposition of the waveform of either Lorentzian, Gaussian or hybrid models.
If deconvolution is performed, the integration value obtained from the result can be recorded automatically to the peak information on a spreadsheet.
In order to perform deconvolution, it is necessary to carry out peak pick of the data set first. When a peak pick is performed, the range in which deconvolution is performed is expanded. Deconvolution is performed to all the peaks currently displayed on the display window. However, in the case of the whole data set, a long period of time may be required.

■ To perform deconvolution:

1. Select **Options**–**Peak**–**Deconvolve** from the menu of the right mouse button, and turn ON the display of the deconvolution.
2. Select **Peak** mode from the cursor tool.
3. Select either **Fit Lorentzian**, **Fit Gaussian** or **Fit Mixed** from the button. In **Peak** mode of the cursor tool, and specify a peak shape.
   When you select a peak shape, deconvolution is simultaneously started.
   Deconvolution is performed under iteration conditions. The $\chi 2$ value (Chi Square) which shows the optimization result is displayed on the **Delta Console** window. Optimization is repeated until the $\chi 2$ value becomes fixed.
   The calculated peak is displayed in yellow. The spectrum of the difference between the spectrum composed from the calculated peak, and the measured spectrum is displayed in red.
4. When displaying the combined spectrum, select **Options**–**Peak**–**Deconvolve Sum** from the right mouse button menu.
   The combined spectrum of the calculated peak is displayed.

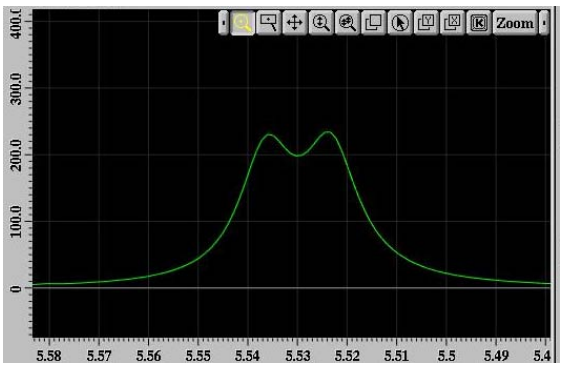


Fig. 2.14 Data before the deconvolution (observation spectrum)

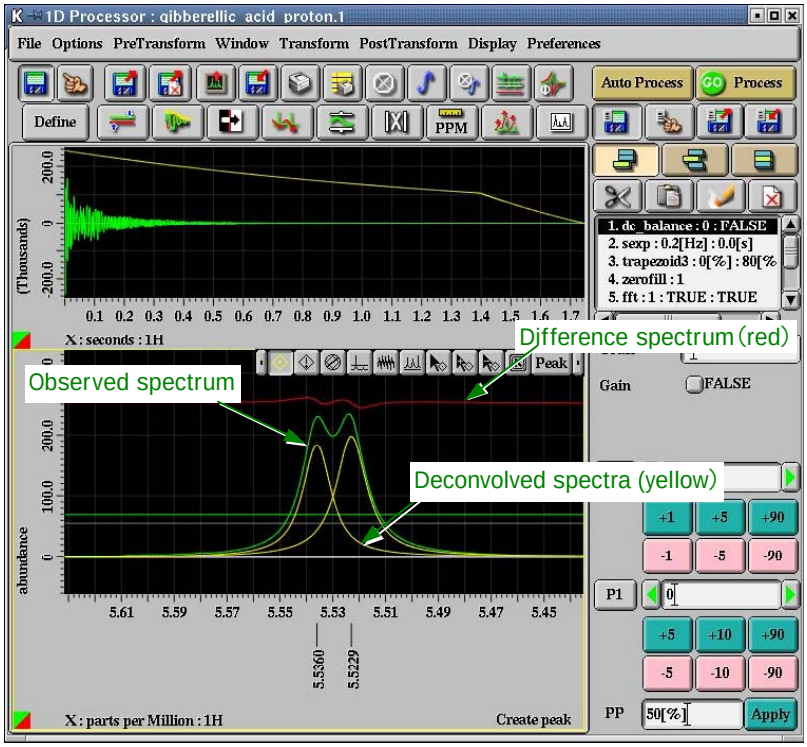


Fig. 2.15 After the deconvolution

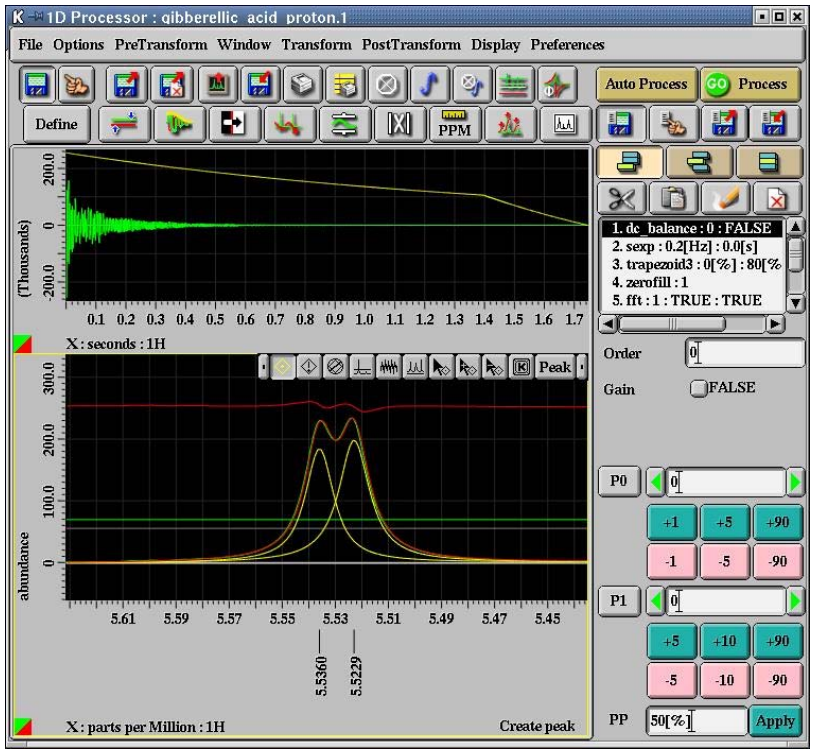


Fig. 2.16 Combined spectrum (Deconvolve Sum)

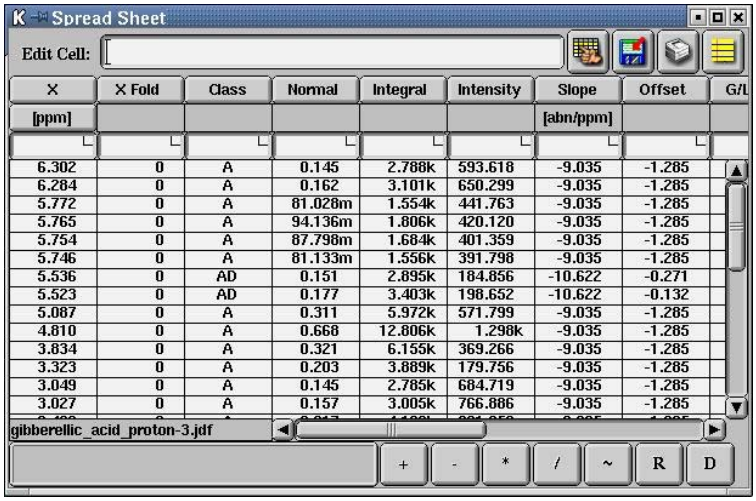
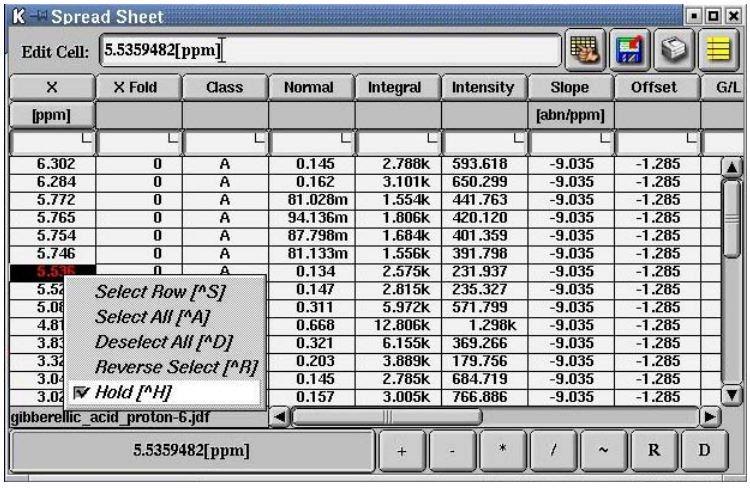


Fig. 2.17 Spread sheet after deconvolution

■ To fix a peak position and perform deconvolution:

1. Display the Spread Sheet.

2. Right-click on the fixed peak, and place a check mark to **Hold**.



3. Perform deconvolution.

The result of the deconvolution which fixed the peak position is displayed.

■ For adding a peak

1. Click on the **Create peak** button in the **Peak** mode of the cursor tool.

2. Left-click on the target peak.

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2D NMR DATA PROCESSING

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3.1 nD PROCESSOR WINDOW

3.1.1 Composition of the nD Processor Window

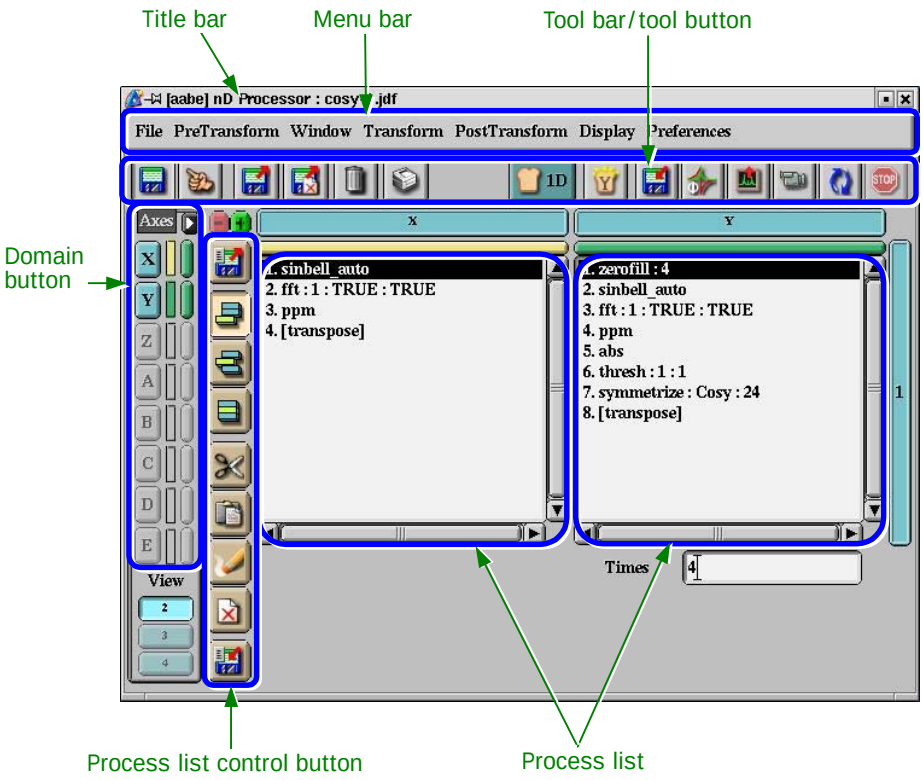

Fig. 3.1 nD Processor window

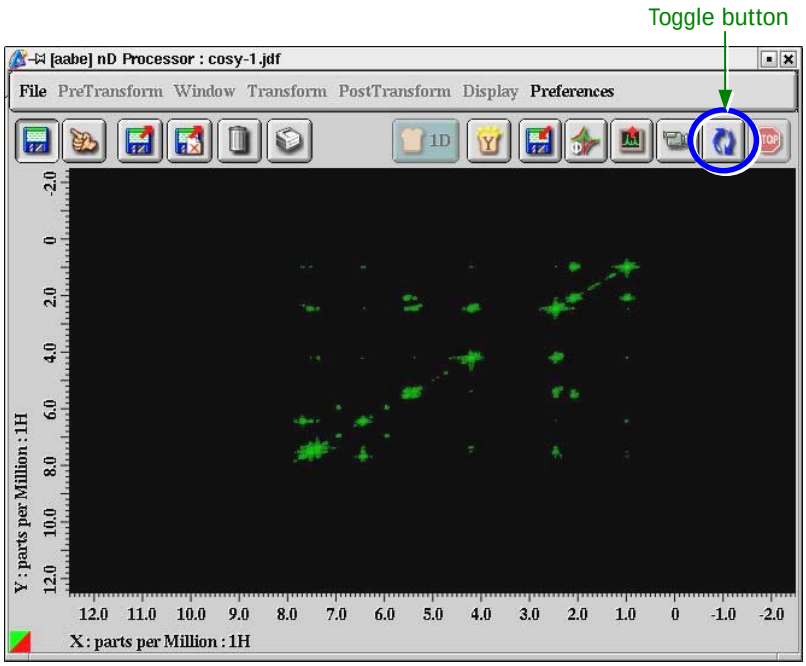
Toggle button
[aabe] nD Processor : cosy-1.jdf
File PreTransform Window Transform PostTransform Display Preferences
1D
Y : parts per Million : 1H
X : parts per Million : 1H

Fig. 3.2 nD Processor window (after data processing)

In the **nD Processor** window, display of the process list of before data processing can be changed using the toggle button to display of the processing result using a list.

Tool bar

The buttons for reading of a data file, saving processing data, and printing are provided in the tool bar on the top of the **2D Processor** window.

Button	Button name	Explanation
	Open Data From Disk	When data is read from a hard disk, this icon is used.
	Open Data By Fingering a Geometry	When data is read from an already opened window, this is used. For example, when reading data from window A to window B, if you select the button in window A, and click on the button, the mouse pointer changes to the finger. Move the mouse button to window B, and click on a data that you want to move. This is the reverse logic to cut & paste.
	Open Data File	Reads in new data to the currently open **nD Processor** window. If the process list the already set up, the contents are immediately adapted for the read data.
	Open Data File and Clear Processing Lists	Reads new data to the currently open **nD Processor** window. At this time, the present process list is deleted.
	Remove File and Clear Processing Lists	Deletes the data currently opened and the process list.
	Print Data	Prints the processing data.
	1D slice on the selected axis with the list in the selected level	Makes 1D slice at the specified position in the selected domain, and displays it on the **1D Processor** window.
	Will process data and put up to sixteen Y slices into Data Slate	Makes 16 slices at the specified positions, and displays them on the **Data Slate** window**.**
	Process File and Save To Disk	Saves the processing data to a hard disk. Data is saved with the same file name and a new version number.
	Process File and Put in 2D Phaser	Performs data processing according to the process list, and displays the results on the **2D Phaser** window.
	Process File and Put in Data Slate	Performs data processing according to the process list, and displays the results on the **Data Slate** window.
	Process File and Put in Data Viewer	Performs data processing according to the process list, and displays the results on the **Data Viewer** window.
	Toggle between processing list view and geometry view	Changes between the process list display screen and the processing result display screen.
	Abort current processing	Cancels processing during data processing.

3.1.2 Domain

Delta treats each axis of NMR data set as a “domain”.
The domain contains the nucleus, the observation range of a spectrum and the processing parameters. The only one domains of an NMR data set can be processed at one time. This is called the “major domain”, other domains are called “minor domains”.
In order to distinguish in the order of evolution times of t_1, t_2, and t_3 in NMR data Delta expresses domain with notation such as x, y, z, α, β, γ, δ, and ε. The x domain is an axis always acquired in the receiver of a spectrometer, which expresses the evolution time domain time in which x, y and z follow in order.
Processing is performed only to the major domain of a data set. Both a major domain and a minor domain can be replaced using the **transpose** command. If the **transpose** command is executed n times for n-dimensional data, a major domain will return to the first domain.

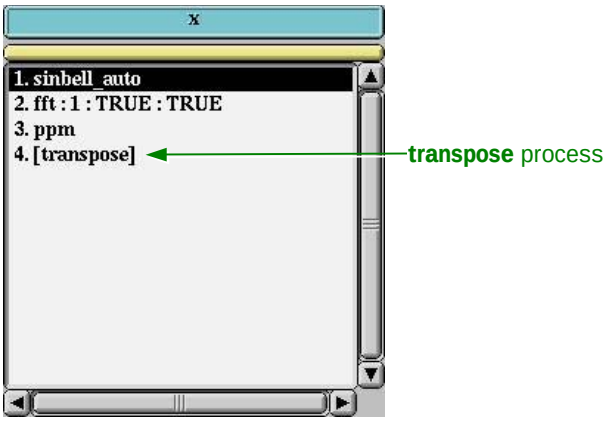

Fig. 3.3 transpose process

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3.1.3 Process List

Chapter 1 explains the fundamental usage of the process list. Although the fundamental function of the process list of two-dimensional (multi-dimensions) data is the same as that of a 1D process list, this section explains a required function using the process list of two-dimensional (many dimensions) data.

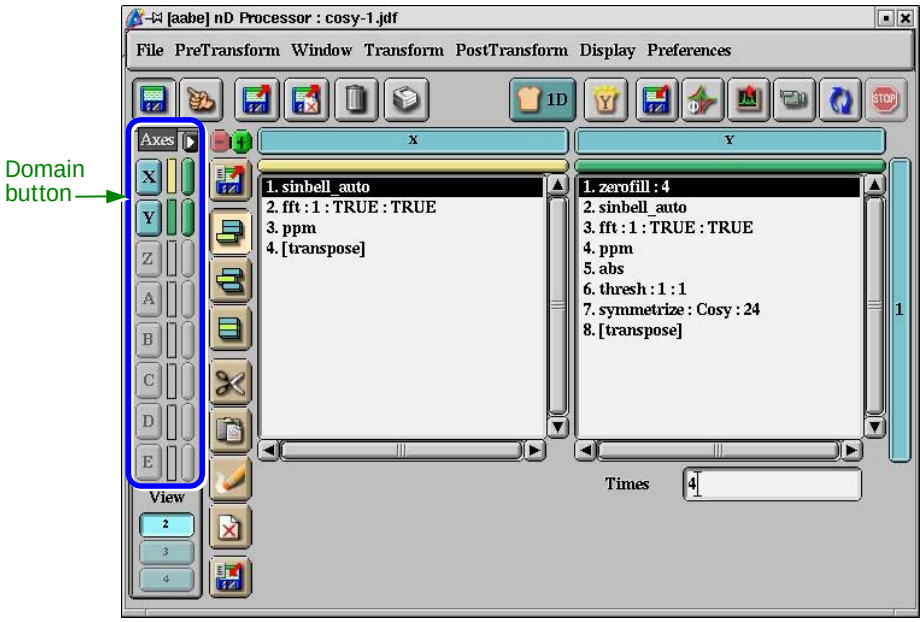
A process list can be written for each domain of a multi-dimensional data set. It is called a “domain list”. Each process list is finished at the **transpose** command. If this **transpose** command is used, a major domain can be changed before processing the next domain. The **transpose** command as well as the **display/phase** command of the **1D Processor** window cannot be deleted from the list.

■ Selecting an active domain

When selecting a domain in the **nD Processor** window, do the following.

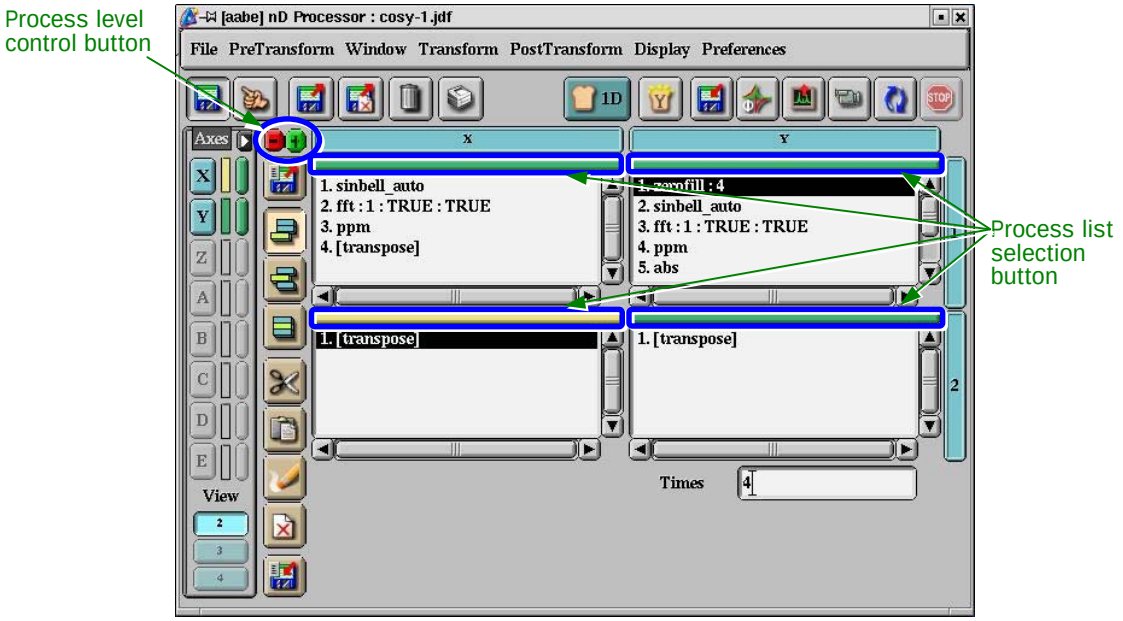
◆ Click on the domain button on the left side of the window.

This is called “selection of an active domain”. Processing is performed only to the selected active domain.



3.1.4 Process Level

After finishing the data processing of each domain, further processing can be performed on the data. Processing is performed from the top to down after finishing the 1st step of processing, processing moves to the 2nd step. A process list is added using the plus button of the process level control button, and deleted using the minus button. Up to 4 levels of a process list can be added. A list can be selected by clicking on the green bar on top of each list. The process list selected changes the color of the bar to yellow. The 2nd list of the X-axis is selected in this example.



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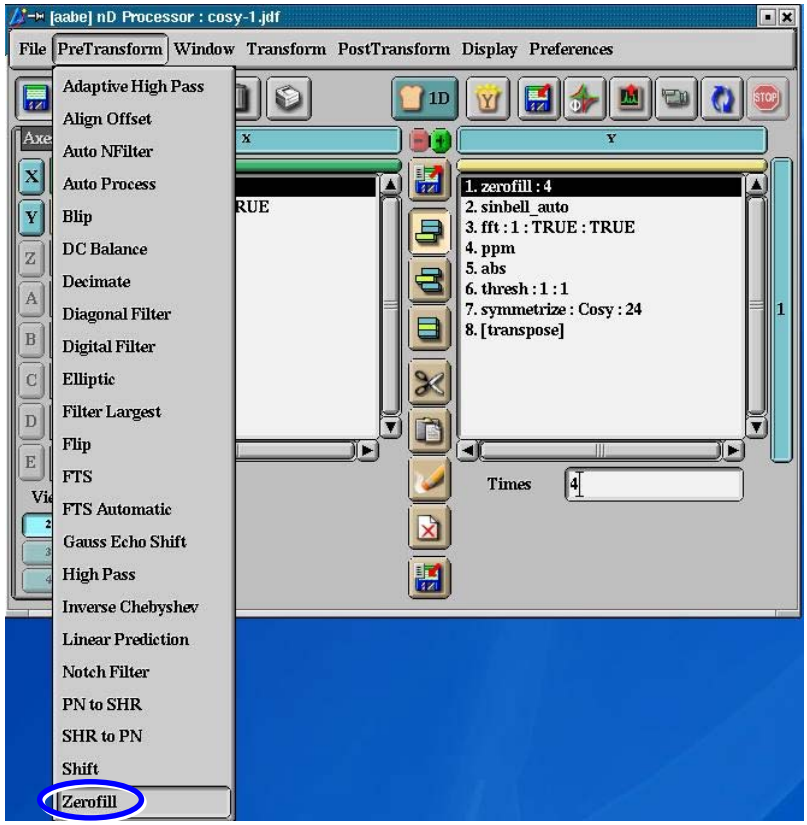
3.2 2D DATA PROCESSING

This section explains the flow of two-dimensional NMR data processing.

3.2.1 Zero Fill

The **Zerofill** function extends the data set by refilling zero data of the scale factor specified an the original data. Since the data size of every dimension consists of the *n*th power of 2, the specified number must be the *n*th power of 2 such as 1, 2, 4, 8, and 16.
If you enter the numerical value that is not the *n*th power of 2, the numerical value of the power of 2 larger than the entered value will be applied.

1. Select the domain that adds the **zerofill** process to the **nD Processor** window.
2. Select **PreTransform**–**zerofill** in the menu bar of the **nD Processor** window.



The **zerofill** process is added to the process list.
In zerofill processing, one argument is attached to a process. This argument is displayed in the **Times** input box.

3. Enter the scale factor of data.

✍ **1** entered in **Times**, mean zerofill is not performed to the data.

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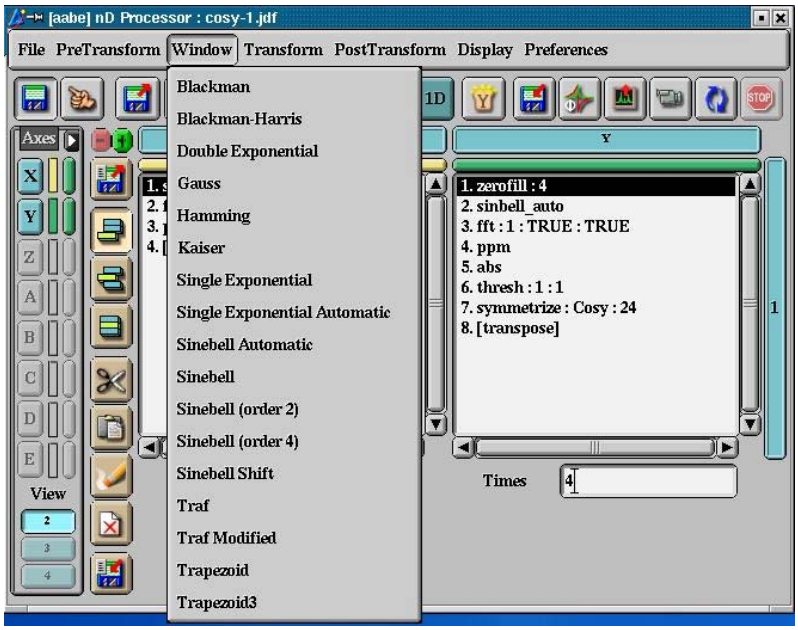
3.2.2 Window Function

Multiplication of a window function is used when emphasizing features, such as resolution enhancement and increasing the signal-to-noise ratio.

3.2.2a To Set a window function:

1. Select the domain which adds a window function in the **nD Processor** window.
2. Select arbitrary window functions in **Window** of the menu bar in the **nD Processor** window.



The window functions are added to the process list.
In a window function, some arguments are attached to the process. These arguments are displayed in the parameter input box.

3. Enter a parameter to the input box.

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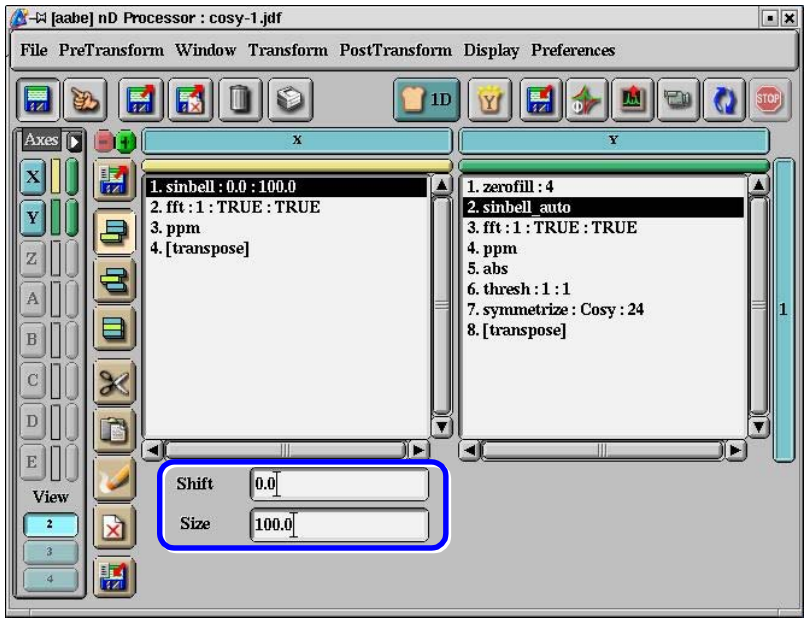
3.2.2b Changing the parameters of a window function

1. Select the domain that changes the parameters in the **nD Processor** window.
2. Select the window function in the process list.
   The window function is highlighted.
   An input box is displayed under the process list display area.

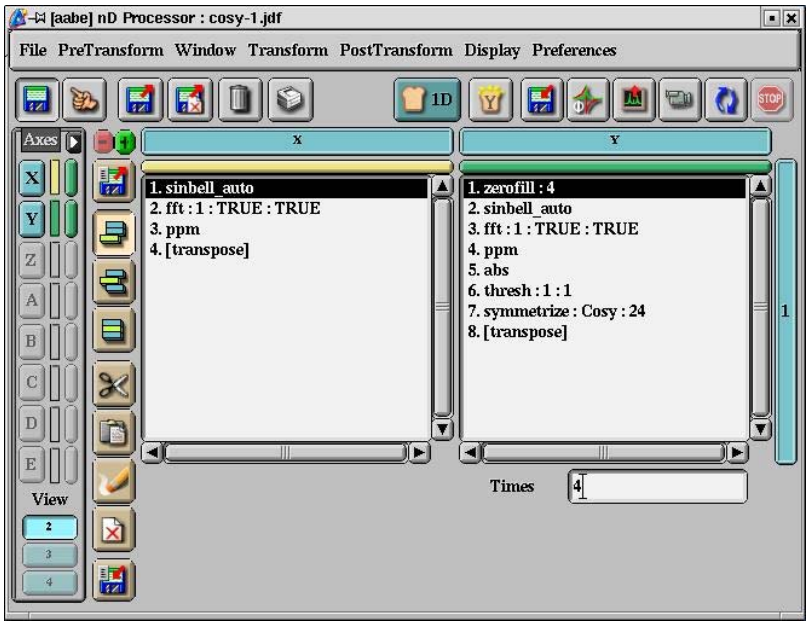


3. Change the numerical value of the parameter of the displayed window function using the keyboard.
4. Click on the Toggle between processing list view and geometry view button.
   Re-processing of the process list is performed, and the result is displayed.
5. Verify the change for a spectrum.
6. Decide on the optimum parameter value while repeating steps 3 to 5.

   A 1D slice data is taken using the **1D slice-the selected axis with the list in the selected level** button, the window function can be evaluated for one-dimensional NMR data, and the parameter can be optimized.

3.2.2c Changing a window function

1. Select the domain that changes the window function in the **nD Processor** window.
2. Select the window function in the process list:



The window function is highlighted.

3. Click on the **Change** button.
4. Select the target window function from the **Window** menus in the menu bar.
   The window function of the process list changes to the selected window function.
5. Click on the Toggle between the processing list view and geometry view buttons.
   Re-processing of the process list is performed, and the result is displayed.
   Change the parameter value of the selected window function if necessary.

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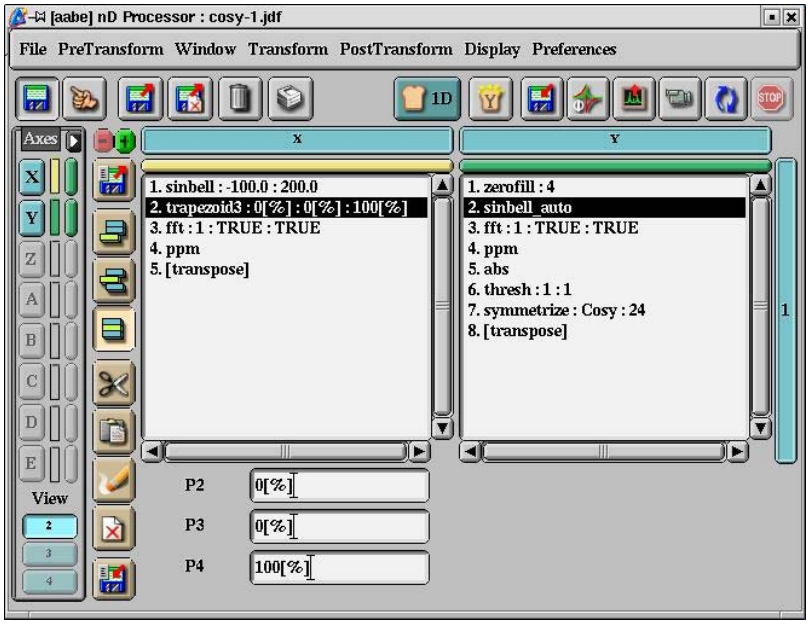
3.2.2d Setting up two or more window functions

Two or more window function can be set up. Setting up is performed separately. The results are multiplied. The multiplication can be applied to input data.

1. Select the domain which adds a window function from the **nD Processor** window.
2. Click on the window function in the process list.



The window function is highlighted.

3. Click on the **Insert** button.
4. Select the target window function from the **Window** menus of the menu bar.
   The selected window function is added to the preceding line above the selected line.
5. Click on the Toggle between processing list view and geometry view button.
   Re-processing by the process list is performed, and the result is displayed.
   Change the parameter value of the selected window function if necessary.

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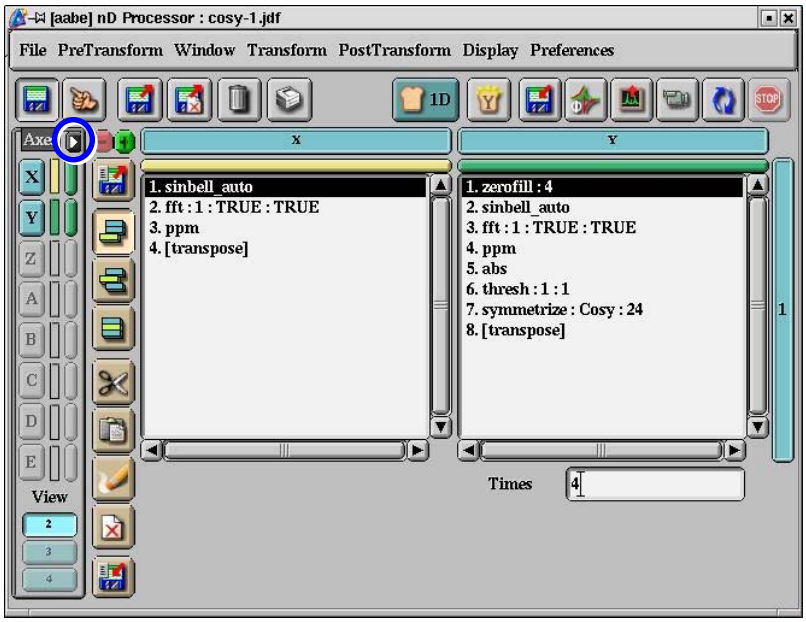
3.2.2e Verifying the window function in one-dimensional slice data

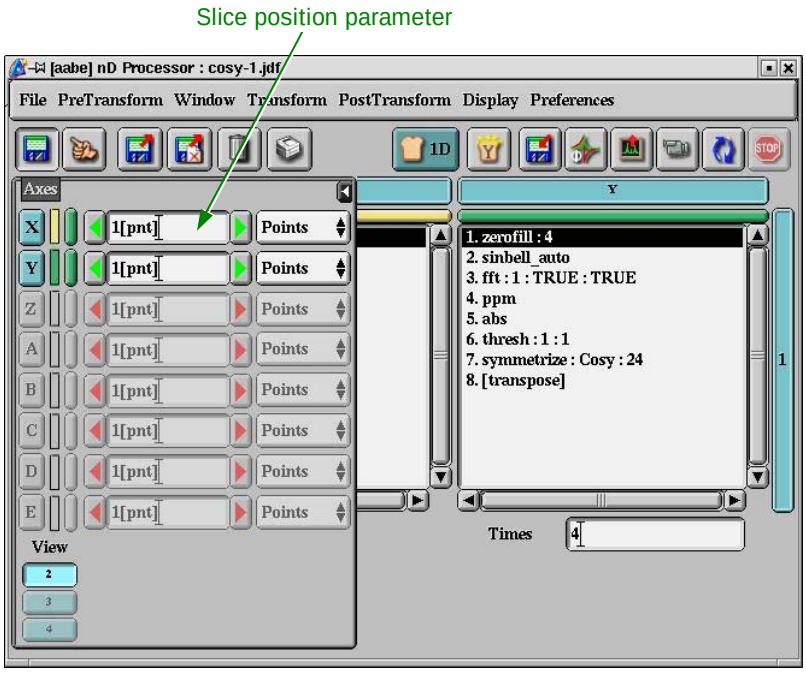
This is the method for checking the set window function using one-dimensional slice data.

1. Click on the **X** or **Y** button for the **Axes** section to select an axis to display.
2. Click on the arrow button of the **Axes** section, and display a slice position parameter.



3. Set up the slice position parameter.

The slice position can be set up by the number of points and %. For example, when calling top X slice data, click on the **X** button to turn ON, and enter 1 **pnt** to the slice position parameter of the Y domain.



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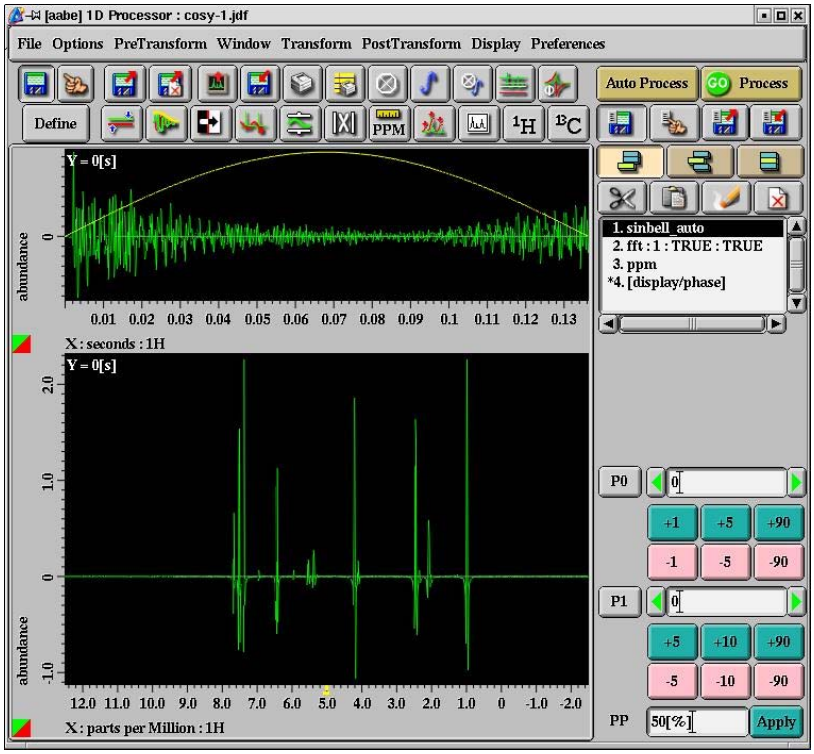
4. Click on the **1D slice-the selected axis with the list in the selected level** button.

The slice data for the position specified in step 3 is displayed in the **1D Processor** window.

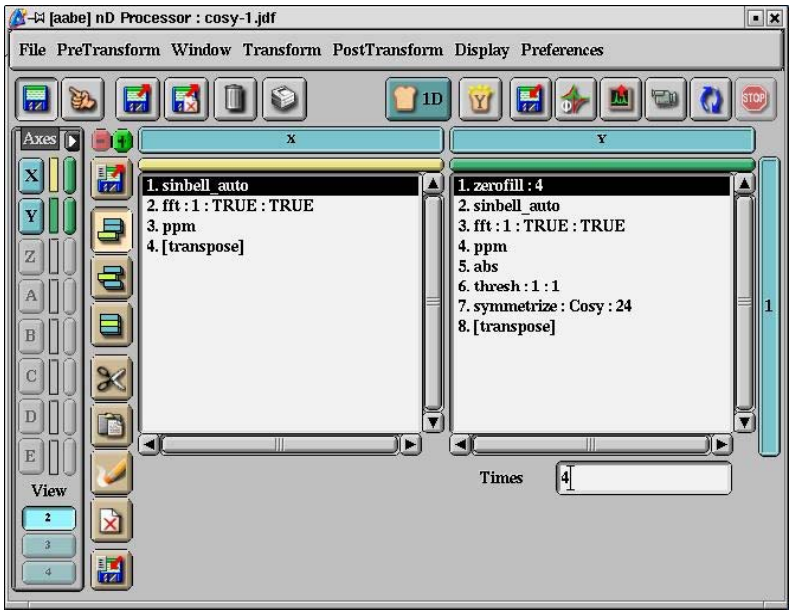


5. Change the window function and parameter value if required.

This is the same operation used to change the window function in normal one-dimensional data.

6. Close the **1D Processor** window.

The window function and parameter which were changed in step 5 are automatically set to the process list of the **nD Processor** windows.



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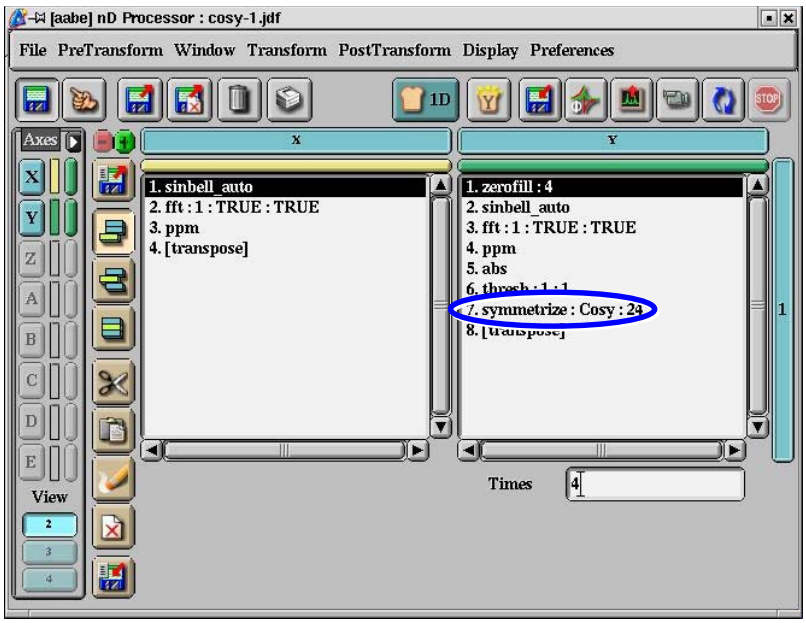
3.2.3 Symmetrization

There are two methods of symmetrization as described below. Symmetrization is useful for reducing asymmetric noise; but if symmetric noise exists, noise may remain in the spectrum just like peaks after symmetrization.

- Apply symmetrization to 2D data in the processing list in a **nD Processor** window before performing an FFT.
- Apply symmetrization to 2D data in the **2D Viewer** window or the **Data Slate** window after performing an FFT.

■ To apply symmetrization to 2D data in the processing list in a nD Processor window before performing an FFT

1. Click on the **Append** button.
2. Click on the **Y** button.
3. Select **PostTransform**–**Symmetrize** from the menu bar.
   Symmetrize is appended to the Y-axis processing list.



4. Set the symmetrize parameters **Type** and **Threshold**.

   Type Select the data type according to the axis of symmetry.

   Threshold Set the standard value to 24.

5. Click on the Process File And Put In Data Viewer button or the Process File And Put In Data Slate button.
   The jobs in the processing list are executed.
   If you click on the button, the **2D Viewer** window appears after processing is complete.
   If you click on the button, the **Data Slate** window appears after processing is complete.

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To apply symmetrization in the 2D Viewer window or the Data Slate window to 2D data after performing an FFT

1. Select **Analysis**–**Symmetrize** from the menu bar in the **2D Viewer** or **Data Slate** window.

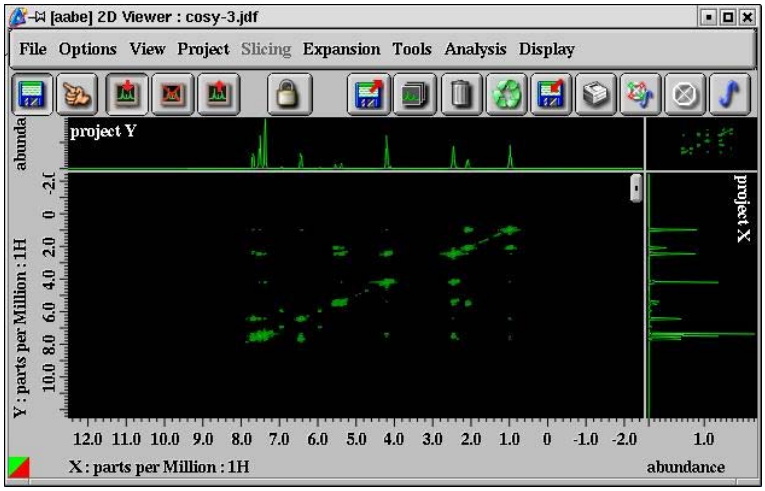

[aabe] 2D Viewer : cosy-3.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
project X
Y : parts per Million : 1H
X : parts per Million : 1H
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0

Fig. 3.4 2D Viewer window

2. Since the pull-down menu is displayed, select an item for a data type.

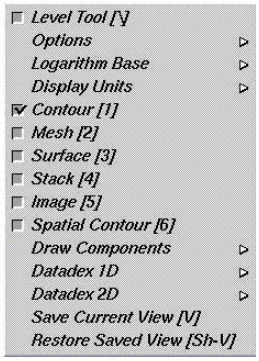
   Symmetrization is performed.

3.2.4 Adjusting Contour Line Display Level

Change the contour line display level after 2D NMR data display is performed in the **Level Tool** window.

1. Select **Select** mode from the cursor tool of the process data display area in the **2D Viewer** window.
2. Click on the **Select geometry** button in the **Select** mode.

3. Move the mouse pointer to the 2D data display area.
4. Press and hold down the right mouse button.
   The pop-up menu appears.



5. Move the mouse pointer to **Level Tool** in the pop-up menu while holding down the mouse button, and release the mouse button.
   The **Level Tool** window opens.

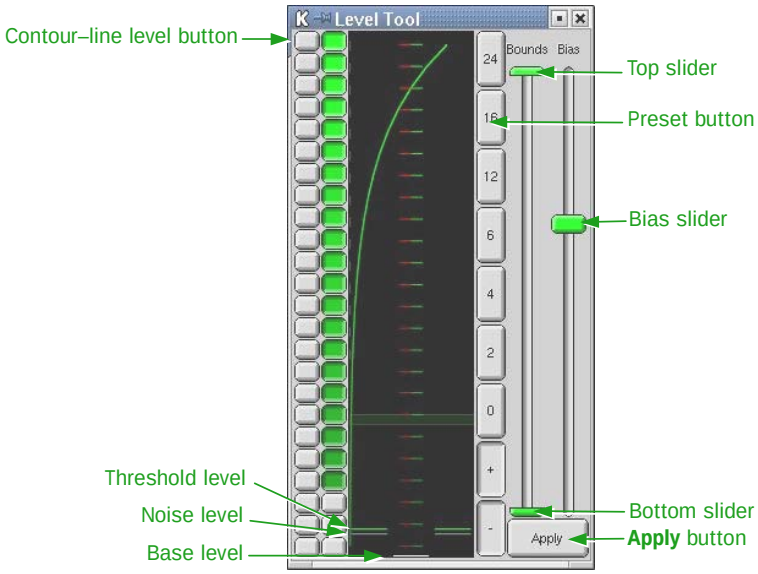
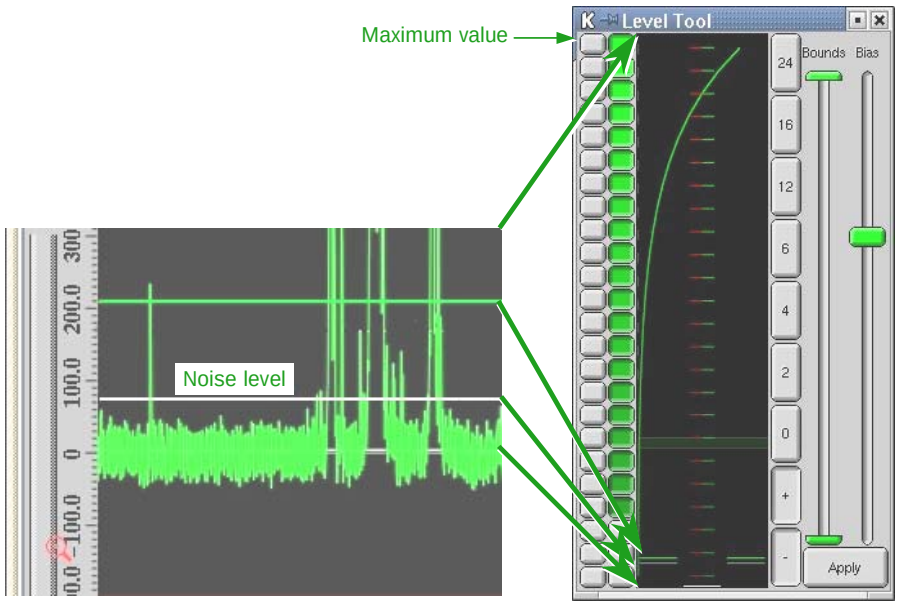


Fig. 3.5 Level Tool window

Button	Explanation
Preset button	Sets the number of contour lines by selecting the 2, 4, 6, 8, 12, or 24 preset button.
Contour-line level button	Specifies the contour level to display by clicking on its button to highlight it.
Top slider	Determines the maximum intensity of the contour lines.
Bottom slider	Determines the minimum intensity of the contour lines.
Bias slider	Determines the signal intensity between the values specified by the top slider (top right) and the bottom slider (bottom left). Moving the bias slider changes the slope of the middle curve shown in figure. Moving it upward results in drawing more contour lines at lower levels of signal intensities.
Noise level	Automatically set after data processing is complete.
Threshold level	Automatically set after data processing is completed, and used for peak picking in 2D processing.
Base level	Zero level for signal intensity. Set it to the lowest level in the **Level tool** window.
Apply button	Clicking on this button redraws the contour lines at the set levels.

6. Adjust the levels of the contour lines in the **Level Tool** window.

Set the minimum intensity based on the noise level. Set the number and intensity of the contour lines to be drawn between the minimum intensity and the maximum intensity in the **Level Tool** window.



Usually, few or no contour lines are set to levels below the noise level. Since setting the contour level below the noise level displays the contour lines of the noise, a large amount of system memory is required, and the processing of the program may become slowing down.

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- **Adjust the levels using the following procedure:**
  - **a.** Turn on the bottom contour-line level button.
  - **b.** Determine the bottom level of the contour lines using the bottom slider.
  - **c.** Determine the top level of the contour lines using the top slider.
  - **d.** Select the number of contour lines you want to display from the preset buttons.
  - **e.** Click on the **Apply** button.

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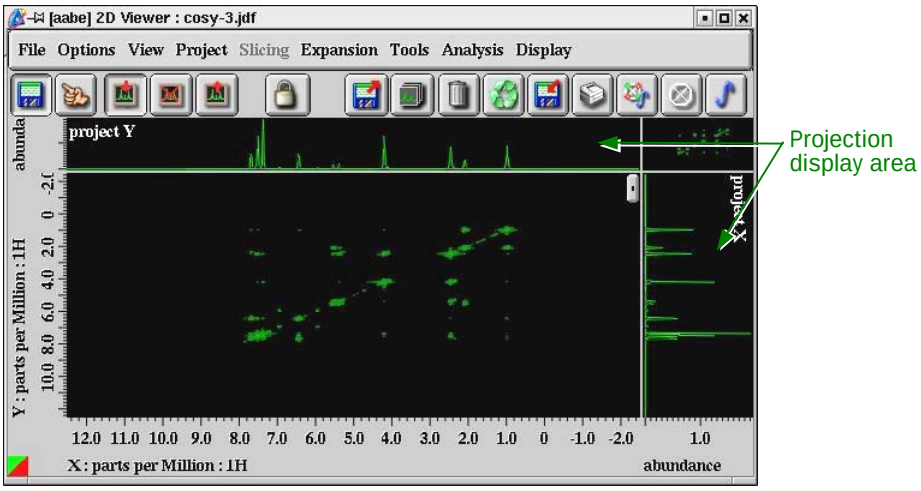
3.2.5 Data Projection

3.2.5a Whole range projection

◆ Select **Project–Full** from the **2D Viewer** window.
Projection data is displayed in the projection data display area.


[aabe] 2D Viewer : cosy-3.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
Projection display area
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

3.2.5b Partial projection

1. Select the **Zoom** mode from the cursor tool bar in the process data display area.
2. Click on the **Zoom Data** button in the **Zoom** mode.
3. Expand the partial projection region using the mouse pointer.
   The expanded spectrum is displayed.
4. Select **Project–Partial** from the menu bar.
   The partial-projection data is displayed in the projection-data display area of the expanded axis. When expanding along the X axis, the part of the data that is expanded is projected onto the X-axis. When expanding along the Y axis, the part of the data that is expanded is projected onto the Y-axis.

Reference: When you select **Display–Row** or **Display–Column** from the menu bar to display the pull-down menu, you can select **Slices**, **Projections**, or **Both**.
If you select **Slices**, only slice data is displayed on the side of the 2D data.

3.2.5c Projection mode

Delta has the following projection mode

Parameter	Value	Explanation
Do Summation	TRUE	Projection in Summation mode.
	FALSE	Projection in Skyline mode (default)
Do Envelope	TRUE	Simultaneous projection for both positive and negative data values is performed.
	FALSE	Simultaneous projection for both positive and negative data values is not performed (default).

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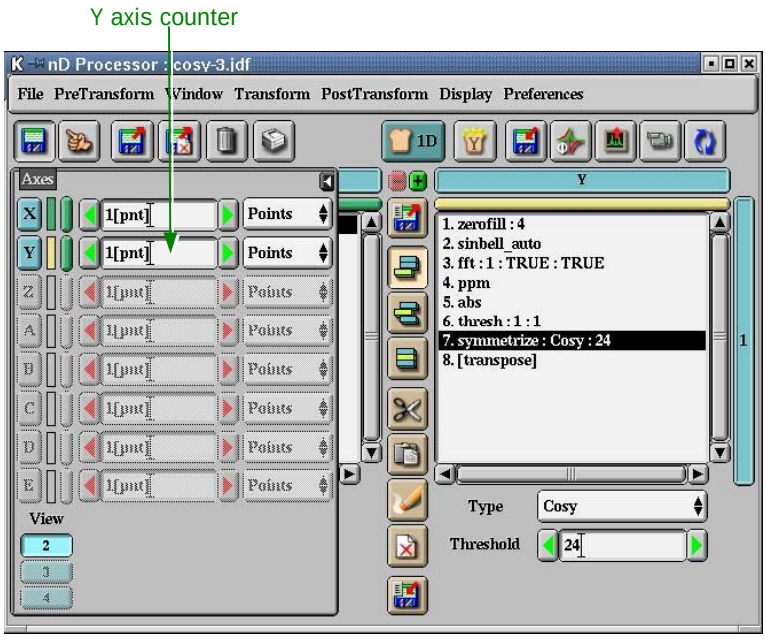
3.2.6 Loading and Processing 1D Slice Data

You can verify a 1D spectrum sliced from multidimensional data set during processing. After you slice 1D data from the multidimensional data set, and process it, you can also reutilize the processing list in multidimensional processing.

3.2.6a Display slice data using a processing list

1. Click on the domain button in the **Axes** section to select the domain.
2. Enter the number of the slice data you want to load in the counter.
   For example, if you want to load the first slice data of the 2D Y axis data, enter 1 in the Y-axis counter.



3. Click on the 1D **1D Slice** button.
   The **1D Processor** window opens, and the slice data specified in the counter is displayed. If the selected domain processing list already exists in the **2D Processor** window, that processing list is copied to the **1D Processor** window and executed.
4. After the **1D Processor** window opens, create a processing list using the same procedure as for 1D data processing.
   If the processing list is already displayed in the **1D Processor** window, correct it.
5. Select **File**–**Close** from the menu bar.
   The **1D Processor** window closes, and the processing list is automatically copied to the **nD Processor** window.

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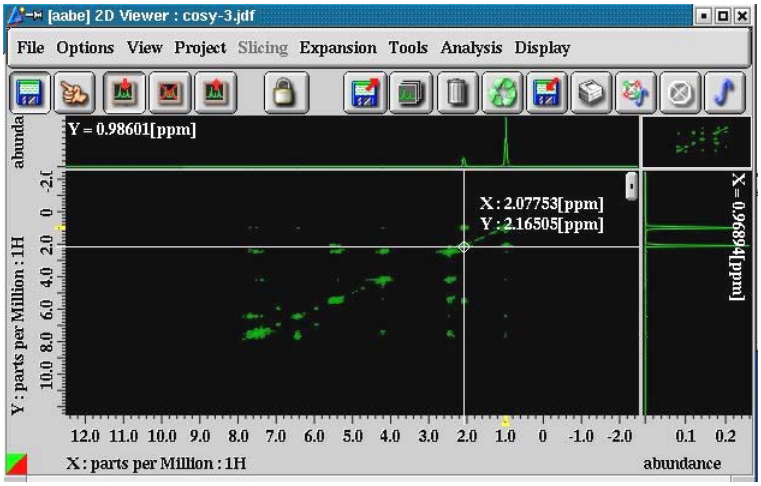
3.2.6b To display slice data in the 2D Viewer window:

1. To display slice data in the projection display area, select **Display**–**Row** or **Display**–**Column** from the menu bar, then select **Slice.**
2. Select the **Pick** mode from the cursor tool bar in the process data display area in the **2D Viewer** window.
3. Click on the **Pick Position** button in **Pick** mode.
4. Move the mouse pointer to the 2D data display area, and press and hold down the left mouse button.
   The slice cursor appears.
5. Move the slice cursor to the slice position while holding down the mouse button, and release the mouse button.


[aabe] 2D Viewer : cosy-3.jdf
File Options View Project Slicing Expansion Tools Analysis Display
Y = 0.98601[ppm]
X : 2.07753[ppm]
Y : 2.16505[ppm]
X = 0.96894[ppm]
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

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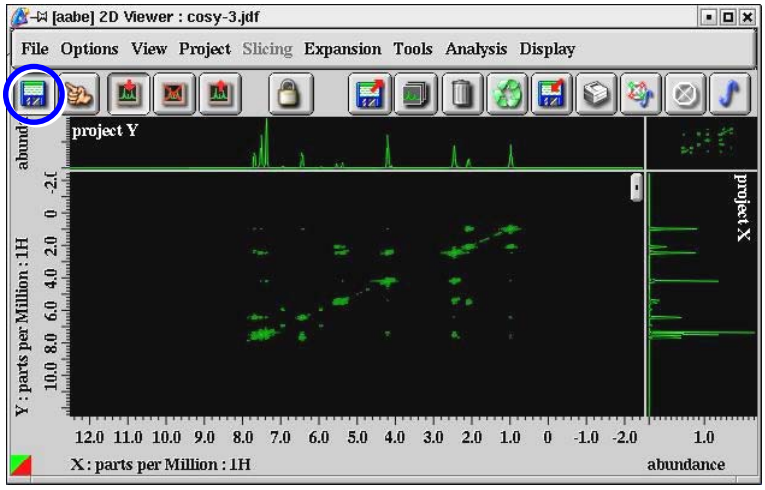
3.2.7 Appending a High Resolution 1D NMR Spectrum

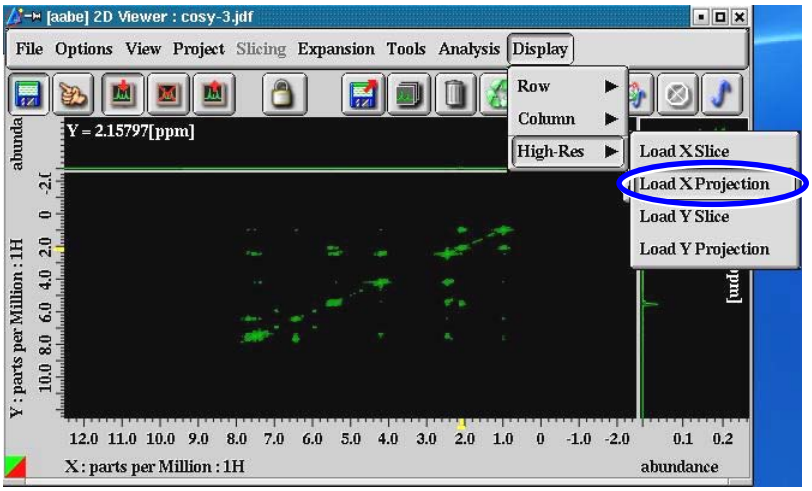
This section explains the method for pasting 1D NMR data on the slice or projection data display area in the **2D Viewer** window.
It is assumed that 1D NMR data for which processing such as FFT has already been completed is saved on the hard disk or displayed in the **1D Processor** window.

3.2.7a To paste data from a disk:

1. Click on the **Open Data From Disk** button.


[aabe] 2D Viewer : cosy-3.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
project X
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

2. Select **Display**–**High-Res**–**Load X Slice** or **Load X Projection**.
The **Open Data for Processing** window opens.



3. Select the file.
1D NMR data is pasted onto the X-axis slice or projection display area.

4. To paste 1D NMR data on the Y-axis display area, repeat Steps 2 and 3.

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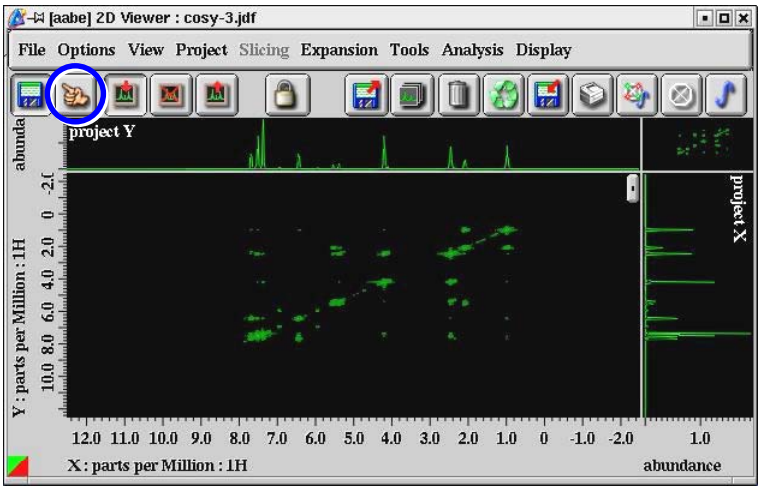
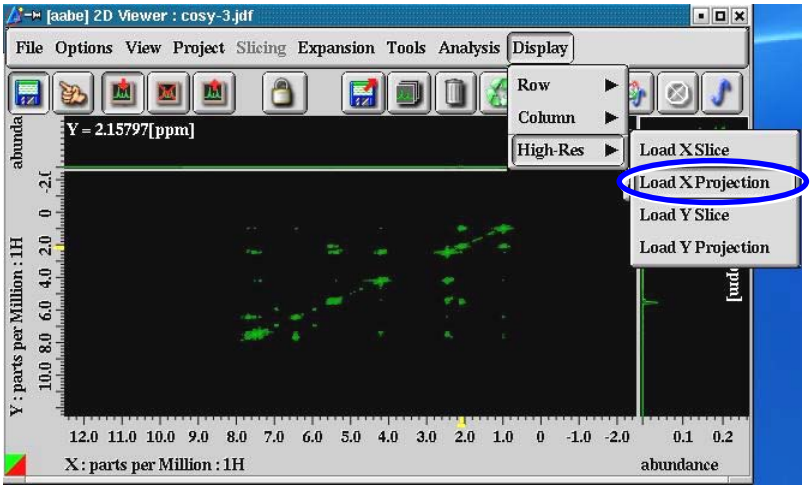
3.2.7b Pasting displayed data

1. Click on the **Open Data by Finger Geometry** button.


[aabe] 2D Viewer : cosy-3.jdf
File Options View Project Slicing Expansion Tools Analysis Display
project Y
project X
Y : parts per Million : 1H
X : parts per Million : 1H
abundance

2. Select **Display**–**High-Res**–**Load X Slice** or **Load X Projection**.
The mouse pointer changes to the finger.



3. Select a spectrum to paste.

4. Pasting 1D NMR data to the Y-axis repeats steps 2 to 3.

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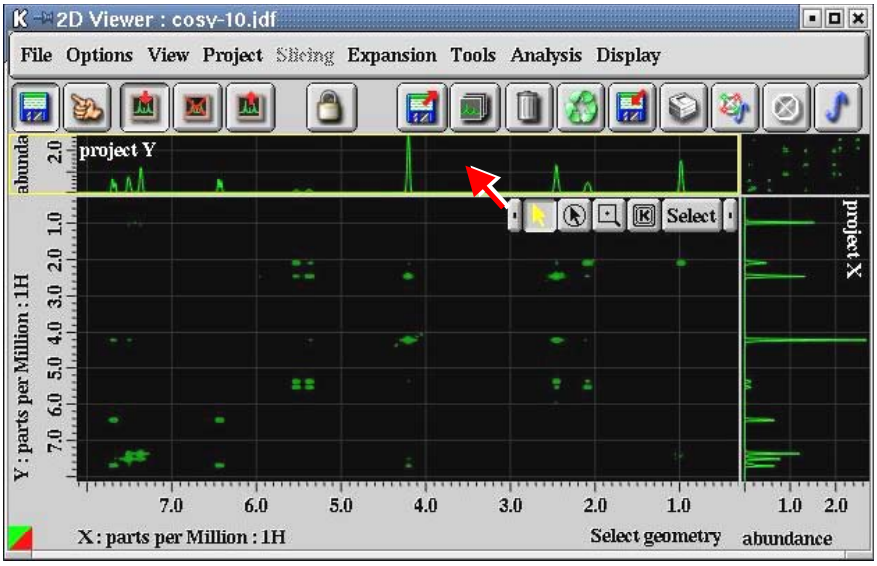
3.2.7c To paste data displayed in another window:

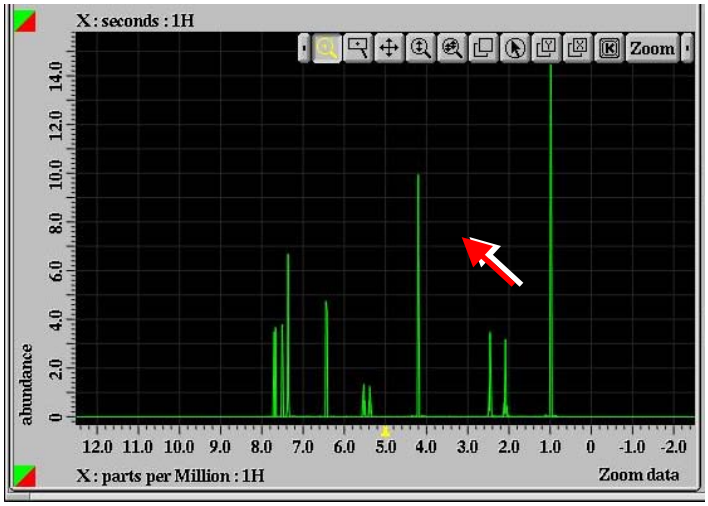
1. Click on the **Key** button in the **2D Viewer** window to open the Key as shown below.

Key button The key button is open.

2. Select the **Select** mode from the cursor tool bar in the process-data display area in the **2D Viewer** window.
3. Click on the **Select geometry** button of the **Select** mode.
4. Move the mouse pointer to the F2-axis projection-data display area or the slice-data display area, on which a 1D spectrum is to be pasted, and click on the left mouse button.



5. Move the mouse pointer onto the displayed 1D spectrum.



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6. Hold down the right mouse button.

The mouse pointer changes as follows:

Mouse pointer

As soon as the mouse pointer changes to the above shape with the right mouse button pressed down, move the mouse pointer quickly.

If you do not move the mouse pointer, a pop-up menu is displayed. If this happens, release the mouse button once, and press and hold down the right button again.

7. Move the mouse pointer, with the mouse button pressed down, onto the **Open Data File** button in the **2D Viewer** window, and release the mouse button.

The 1D spectrum is displayed in the area selected in Step 4.

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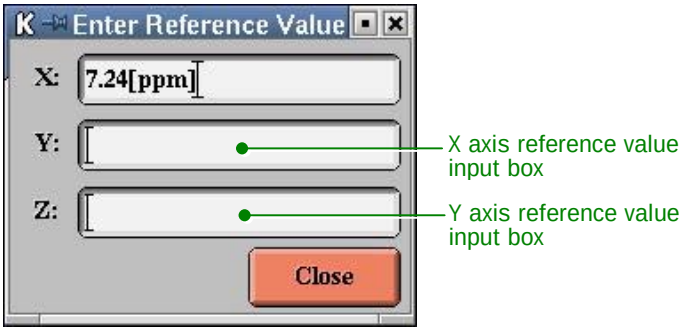
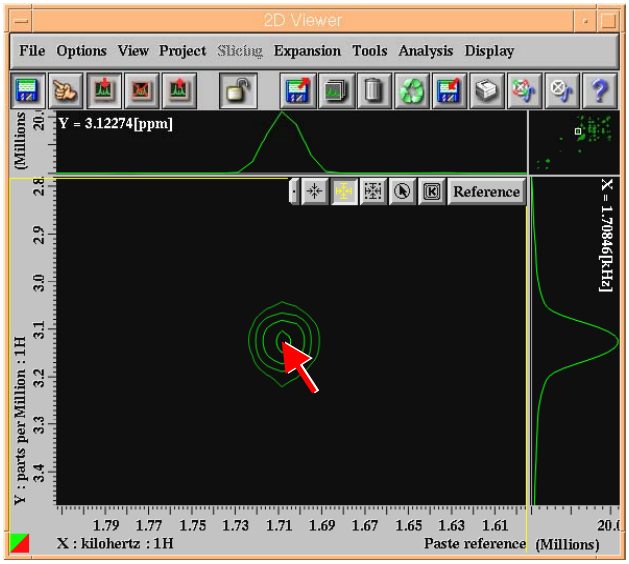
3.2.8 Reference Setting

The reference may be set in the **2D Viewer** or **Data Slate** window.

1. Expand the peak which you want to use as a reference line position.
2. Select **Tools**–**Reference** from the menu bar in the **2D Viewer** or **Data Slate** window.
   The **Enter Reference Values** window opens.



   The **Enter Reference Values** window opens.
3. Enter the reference values in the X-axis reference value input box and the Y-axis reference value input box in the **Enter Reference Values** window.
   The units are the same as those used in the rulers.
4. Select the **Reference** mode from the cursor tool bar in the process data display area.
5. Click on the **Paste reference** button in **Reference** mode.
6. Move the mouse pointer to the peak vertex to set its reference.



7. Click on the left mouse button.
   The position of the clicked peak changes to the reference value set in Step 3.

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3.2.9 Peak Pick

Peak pick is performed in the **2D Viewer** window or the **Data Slate** window.

- Click on the Peak Pick and Integrate button or the Peak Pick and Integrate with Cosy Peak J Width button in the 2D Viewer or Data Slate window.

  The peak pick is executed and the peak marker is displayed.
  When the button is used, a J-split cosy peak is treated as one peak.

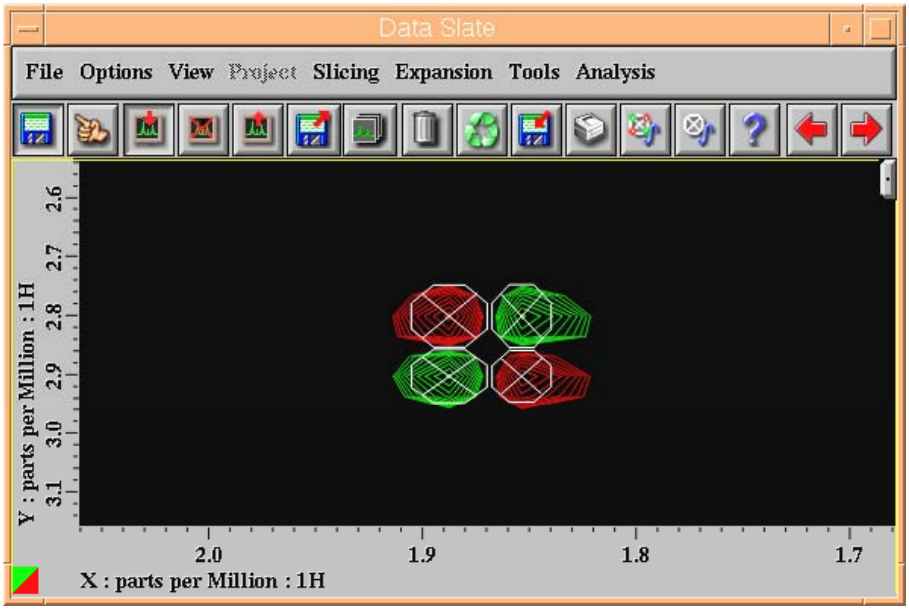

Fig. 3.6 Result of Peak Pick

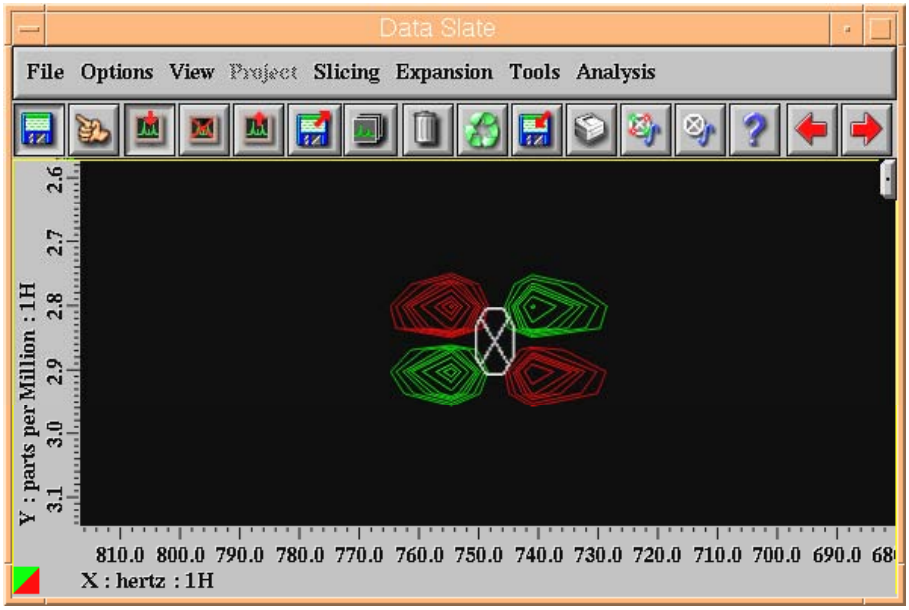

Fig. 3.7 Result of using Peak Pick and integrate with Cosy Peak J Width

When you use the **Peak Pick and Integrate with Cosy Peak J Width** button, you must set the J value. Set it according to the procedure of section 3.2.9a “Setting the J value” (below).

If the number of peaks is not appropriate for peak pick, adjust the threshold and base levels according to the procedure of section 3.2.9b “Adjusting the threshold and base level”(below), and perform peak pick again.

Reference: The detailed result of the peak pick is displayed in the **Spread Sheet** window. Refer to section 3.2.9c “Displaying the peak pick result in the Spread Sheet window”.

3.2.9a Setting the J value

1. Select **Options–Set Cosy Peak J Width** from the menu bar in the **2D Viewer** or **Data Slate** window.
   The **Peak Cosy j Width** window opens.

Fig. 3.8 Peak Cosy j Width window

2. Enter a suitable J value in the J-value input box.

After this operation, perform peak pick using the **Peak Pick and Integrate with Cosy Peak J Width** button. The result of the peak pick depends on the J value you set.

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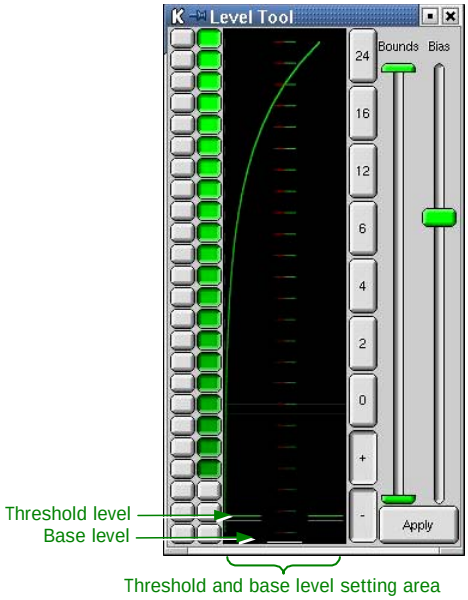
3.2.9b Adjusting the threshold and base levels

If there are too many or too few detected peaks as a result of the peak pick, you must adjust the threshold and base levels.

1. Select the **Select** mode from the cursor tool bar in the 2D process data display area.
2. Click on the **Select geometry** button in the **Select** mode.
3. Move the mouse pointer to the 2D data display area.
4. Select **Level Tool** from the right mouse-button menu.
   The **Level Tool** window opens.
5. Move the mouse pointer to the threshold and base level setting area of the **Level Tool** window.



6. Select **Statistics from** the right button menu.
7. Press and hold down the left mouse button in the threshold and base level setting area.
8. Move the mouse pointer to the position to which you want to set the threshold level while holding down the mouse button, and release the mouse button.
   The threshold level changes.
   After this operation, perform the peak pick. As a result, if you need to adjust the noise level, carry out the following procedure:
9. Move the mouse pointer to the threshold and base level setting area in the **Level Tool** window; press and hold down the middle mouse button.
10. Move the mouse pointer to the position to which you want to set the base level while holding down the mouse button; release the mouse button.
    The base level changes.

After this operation, perform peak pick again.

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3.2.9c To Display the peak pick results in the Spread Sheet window:

1. Click on the **Spread Sheet** button in the **Delta Console** window.
   The **Spread Sheet** window opens.
2. Click on the **Finger Data in Geometry** button in the **Spread Sheet** window.
   The mouse pointer changes to the finger shape.
3. Move the mouse pointer onto the displayed 2D NMR data, and click on it.
   The detailed result of the peak pick is displayed.

☞ For information about the **Spread Sheet** window, refer to Chapter 7 “ How to use the Spread sheet”.

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3.2.10 Data Processing of Phase Sensitive 2D Data

In the case of phase sensitive 2D data, phase-correction processing and positive and negative peak display control are necessary in addition to various kinds of data processing for 2D data in the absolute-value display mode.

3.2.10a Phase-correction processing

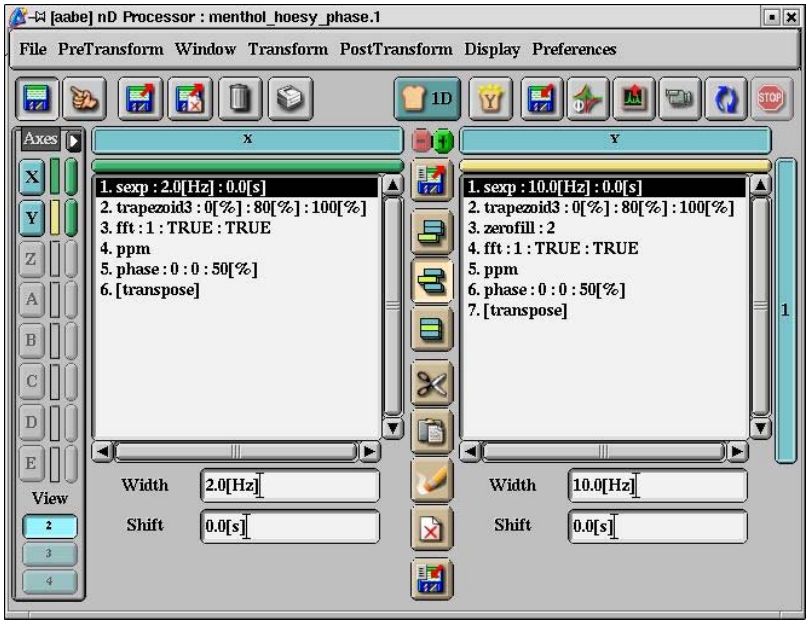
If the appropriate phase-correction values are known in advance, or if the calculated values are used as phase correction values, record phase correction values to the processing list in the **nD Processor** window, and perform phase correction processing.

If the appropriate phase correction values are unknown, perform phase correction processing in the Phase 2D window.

■ If phase correction values are known or calculated values are to be used

If the appropriate phase-correction values are known in advance, or if the calculated values are used as phase correction values, record phase correction values to the processing list in the **nD Processor** window, and perform phase correction processing according to the following procedure:

1. Click on the **Append** button in the **nD Processor** window.
2. Click on the **X** button.
3. Select **PostTransform–Phase–Apply Phase**.
   The process item, **phase:0:0:50(%),** is displayed just before **transpose**.
   The P0, P1, and PP input boxes are displayed under the X-axis processing list display area.


[aabe] nD Processor : menthol_hoesy_phase.1
File PreTransform Window Transform PostTransform Display Preferences
1D
Axes
X
Y
1. sexp : 2.0[Hz] : 0.0[s]
2. trapezoid3 : 0[%] : 80[%] : 100[%]
3. fft : 1 : TRUE : TRUE
4. ppm
5. phase : 0 : 0 : 50[%]
6. [transpose]
1. sexp : 10.0[Hz] : 0.0[s]
2. trapezoid3 : 0[%] : 80[%] : 100[%]
3. zerofill : 2
4. fft : 1 : TRUE : TRUE
5. ppm
6. phase : 0 : 0 : 50[%]
7. [transpose]
Width 2.0[Hz]
Shift 0.0[s]
Width 10.0[Hz]
Shift 0.0[s]
View

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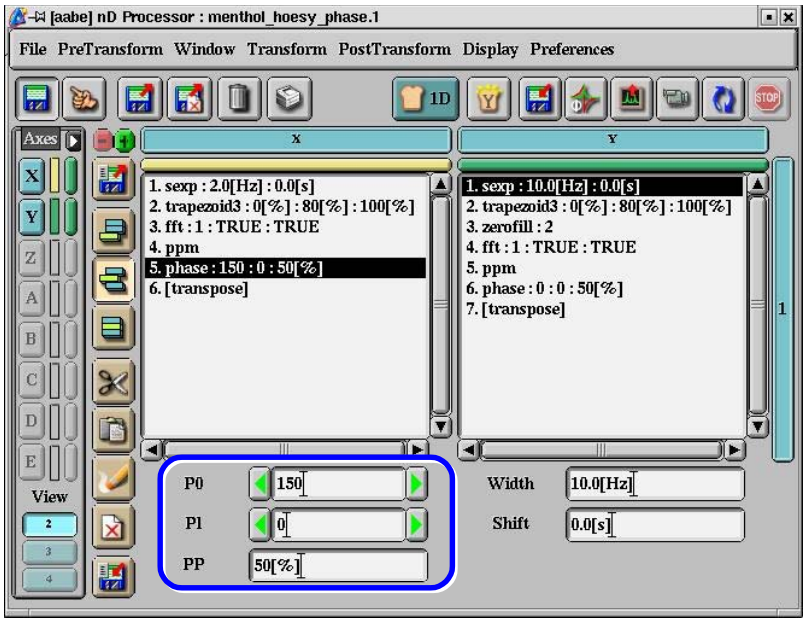
4. Enter the phase correction values in the **P0**, **P1**, and **PP** input boxes.

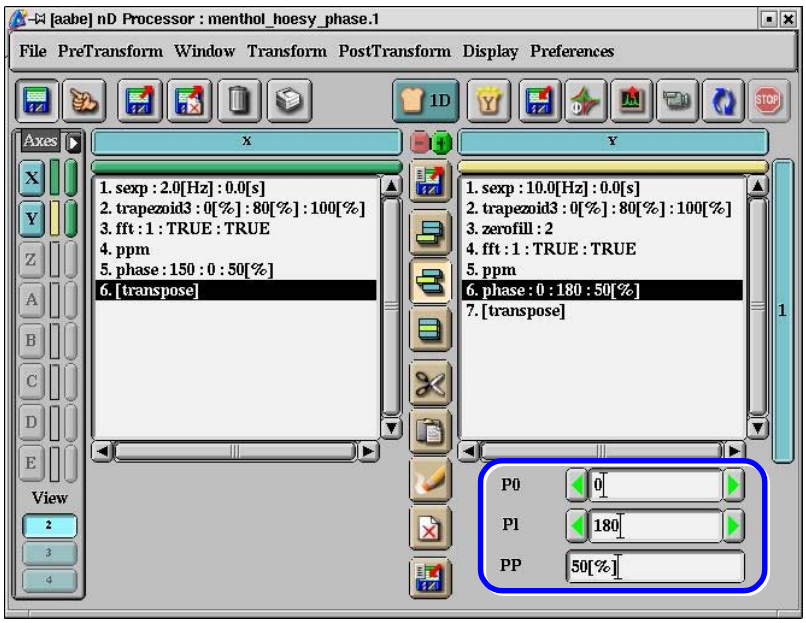

[aabe] nD Processor : menthol_hoesy_phase.1
File PreTransform Window Transform PostTransform Display Preferences
1D
Axes
X
Y
1. sexp : 2.0[Hz] : 0.0[s]
2. trapezoid3 : 0[%] : 80[%] : 100[%]
3. fft : 1 : TRUE : TRUE
4. ppm
5. phase : 150 : 0 : 50[%]
6. [transpose]
1. sexp : 10.0[Hz] : 0.0[s]
2. trapezoid3 : 0[%] : 80[%] : 100[%]
3. zerofill : 2
4. fft : 1 : TRUE : TRUE
5. ppm
6. phase : 0 : 0 : 50[%]
7. [transpose]
P0 150
P1 0
PP 50[%]
Width 10.0[Hz]
Shift 0.0[s]
View

5. Click on the **Append** button in the **nD Processor** window.

6. Click on the **Y** button.

7. Select **PostTransform–Phase–ApplyPhase** from the **nD Processor** window.
   The process item, **phase:0:0:50(%),** is displayed just before **transpose**.
   The P0, P1, and PP input boxes are displayed under the Y-axis processing list display area.

8. Enter the phase correction values in the **P0, P1**, and **PP** input box.


[aabe] nD Processor : menthol_hoesy_phase.1
File PreTransform Window Transform PostTransform Display Preferences
1D
Axes
X
Y
1. sexp : 2.0[Hz] : 0.0[s]
2. trapezoid3 : 0[%] : 80[%] : 100[%]
3. fft : 1 : TRUE : TRUE
4. ppm
5. phase : 150 : 0 : 50[%]
6. [transpose]
1. sexp : 10.0[Hz] : 0.0[s]
2. trapezoid3 : 0[%] : 80[%] : 100[%]
3. zerofill : 2
4. fft : 1 : TRUE : TRUE
5. ppm
6. phase : 0 : 180 : 50[%]
7. [transpose]
P0 0
P1 180
PP 50[%]
View

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9. Click on the Process File And Put In Data Viewer button.

After performing data processing in the process list, the **Data Viewer** window appears.

10. Verify the two-dimensional data after phase calibration is displayed in the **2D Viewer** window.

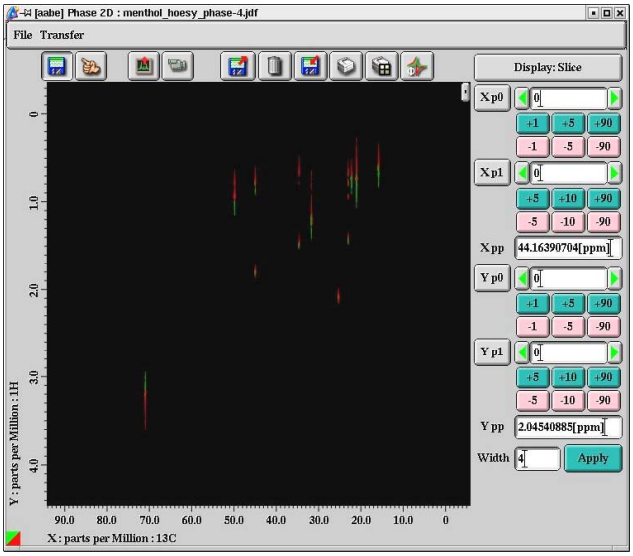
When phase correction is required again because phase correction is not suitable, perform it according to the operation procedure "■ When the suitable phase calibration value is not known" described below.

The units **ppm** and **points** besides **%** are also available for **PP.** However, ppm-unit axis processing is necessary to enter the value in **ppm** before phase correction processing. To enter it in **points,** it is necessary to convert the value, depending on the expansion ratio for zero filling.

When suitable phase correction value is not known

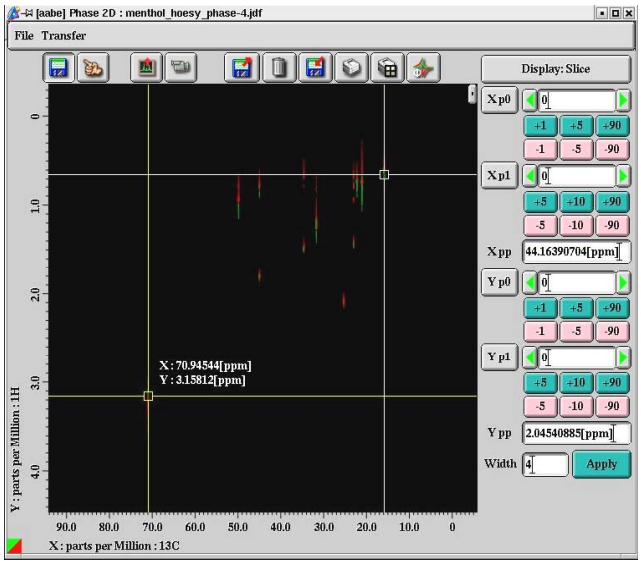
When the suitable phase correction value is not known, calculate the phase correction value from each slice of data using the functions of the **Phase 2D** window after performing 2D Fourier transform processing to perform phase correction processing.

1. Click on the **Phase 2D** button in the **nD Processor** window to set up the required process list.



2. Select the **Cursor** mode from the cursor tool in the two-dimensional data display area.
3. Click on the **Create Cursor** button in the **Cursor** mode.
4. Select chooses two peaks used for phase correction, whose phases still are not completely correct.

   At this time, select two points that as far separate diagonal as possible.



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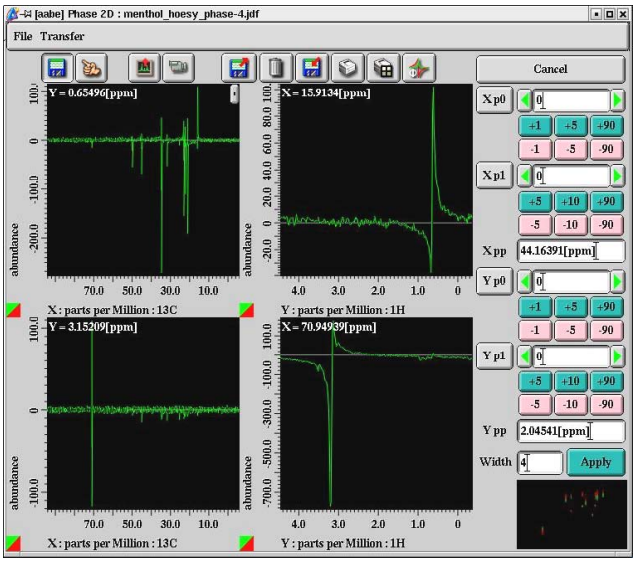
5. Click on the **Display : Slice** button.



6. Select the **Phase** mode from the cursor tool in the X-axis slice data display area of the first point.

7. Click on the **Adjust the Phase PP value** button in **Phase** mode.

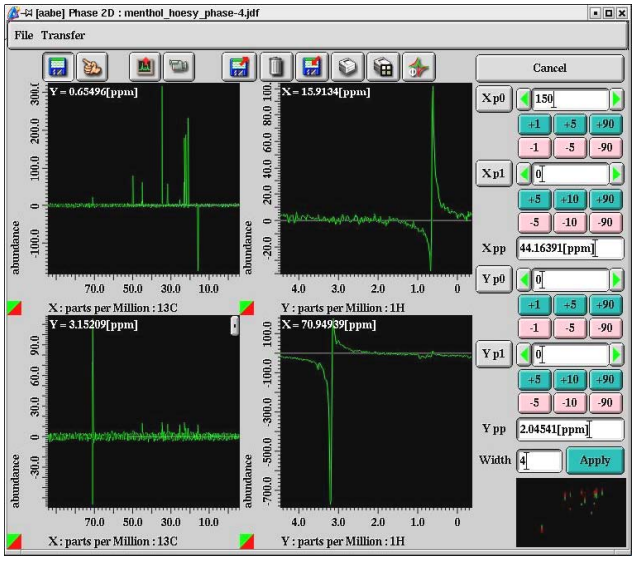
8. Move the mouse pointer to the X-axis slice data display area for the first point; press and hold down the left mouse button.

9. Move the slice cursor to a peak position whose phase adjustment is easy in order to corrects the **P0** of the X-axis while holding down the mouse button, and release the mouse button.

The value of the X-axis at the position that released the mouse button is entered in the **Xpp** input box.

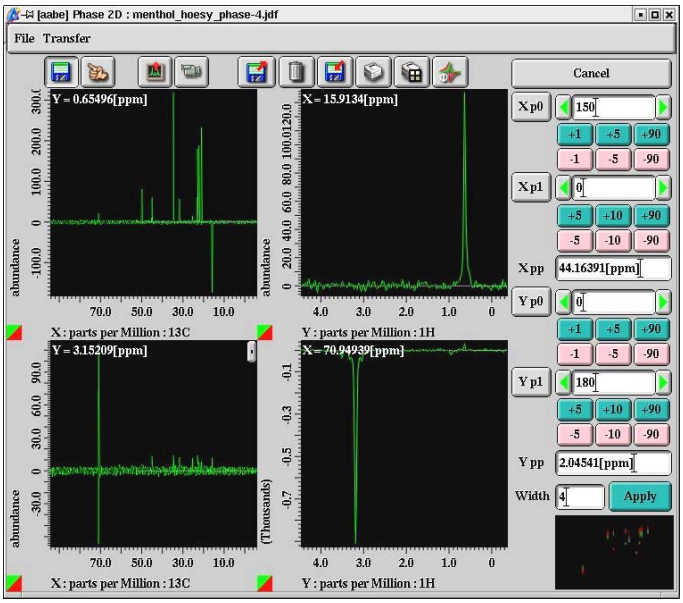
10. Adjust **P0** of the X-axis while viewing the peak of the X-axis slice data at the first point.

11. Adjust **P1** of the X-axis while viewing the peak of the X-axis slice data at the 2nd point.

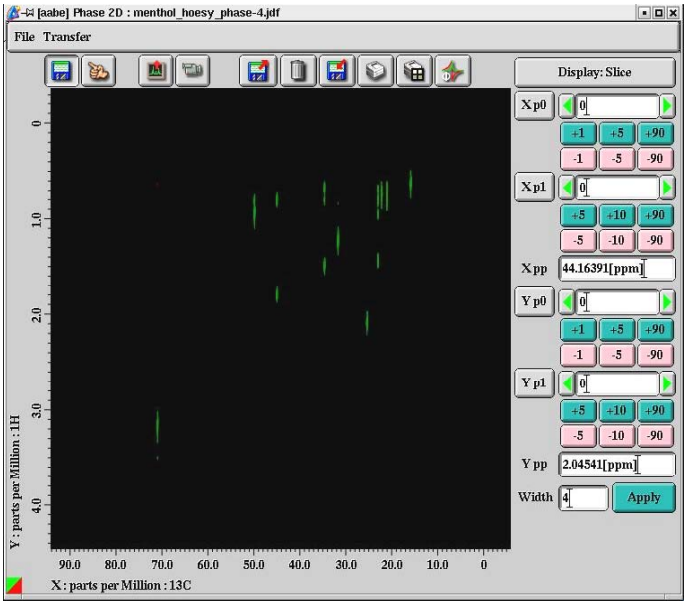


12. Perform phase correction for the Y-axis.

The phase correction for the Y-axis will be performed with the same procedure as phase correction for the X-axis.



13. Click on the **Apply** button.



14. Click on the **Move Data to 2D Viewer** button or **Move Data to Data Slate** button to display the two-dimensional data corrected phase on the **2D View** or **Data Slate** window.

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3.2.10b Positive and negative peak display control

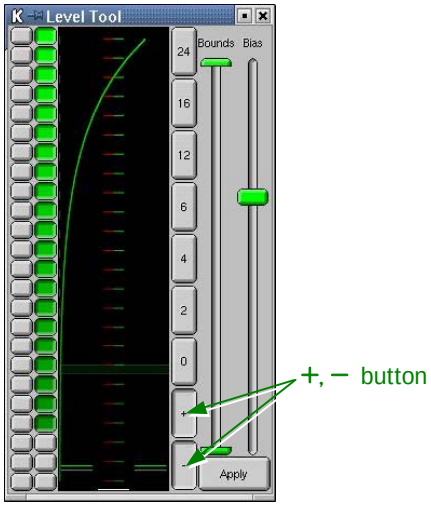
There is 2D phase-sensitive data only for positive peaks in after phase correction processing is complete. In this case, only positive peaks are displayed.
Moreover, only positive or negative peaks may need to be plotted. In this case, only positive or negative peaks are displayed.
Control of positive and negative peak display is performed in the **Level Tool** window.

■ Level tool display

1. Select the **Select** mode from the cursor tool in the processing data display area in the **2D Viewer** window.
2. Click on the **Select geometry** button in the **Select** mode.
3. Move the mouse pointer to the two-dimensional data display area.
4. Select **Level Tool** from the right button menu.
   The **Level Tool** window opens.

■ To display only positive peaks:

◆ Click on the minus (–) button in the **Level Tool** window to turn it off.
Only the positive peaks are displayed.



Turning on the minus (-) button by clicking on it again displays negative peaks.

■ To display only negative peaks:

◆ Click on the plus (+) button in the **Level Tool** window to turn it off.
Only the negative peaks are displayed.
Turning on the plus (+) button by clicking on it again displays the positive peaks.

C I

3.2.11 Other Processing

For information about comments, PIP, spreadsheets, spectral display settings, and plotting, refer to Chapter 2 “ 1D Data Processing”.

If you turn on **Negative Contour Grey** using a monochrome printer, the negative contour lines are plotted with broken lines.

You can change the setting of a **Negative Contour** from the **Printer** tag in the **References Tool** window by selecting **File–Preferences** in the **Delta Console** window.

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4

ARRAY DATA PROCESSING

4.1 OUTLINE OF ARRAY MEASUREMENT DATA PROCESSING 4-1
4.2 PROCESSING METHOD FOR ARRAY MEASUREMENT DATA 4-2
4.2.1 Processing as a Single Data File 4-2
4.2.1a When process conditions are saved in the processing list 4-2
4.2.1b When the processing list is not provided 4-4
4.2.1c Displaying data in the Data Slate window 4-7
4.2.2 Processing Data taken from the Measurement Data Sets 4-8

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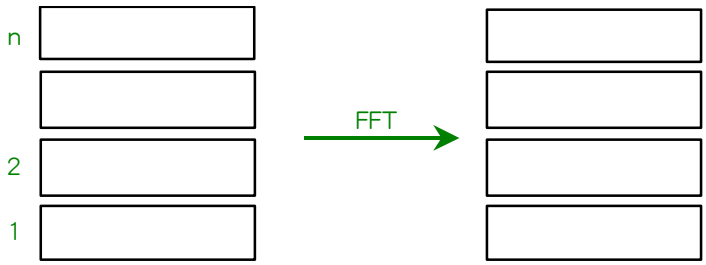
4.1 OUTLINE OF ARRAY MEASUREMENT DATA PROCESSING

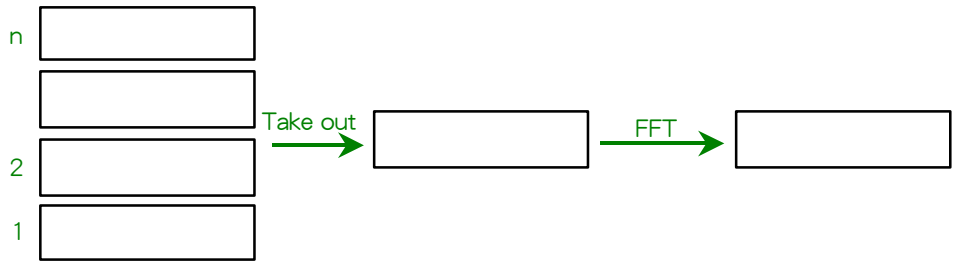
Array measurement data is the data set obtained when the one–dimensional data, such as relaxation time measurement data or multi-dimensional data obtained while changing conditions by continuous measurement are saved in a file.
Therefore, similar data processing using multi-dimension NMR data will be performed using **nD Processor or Data Slate.**
Moreover, in relaxation time measurement or diffusion measurement data processing, data analysis is performed using the **Curve Analysis Tool**.

Two methods of array measurement data processing follow:

- Processing all measurement data sets from the first to the nth together under the same conditions:



Processing one set of data obtained from the first to the *n*th measurement data sets



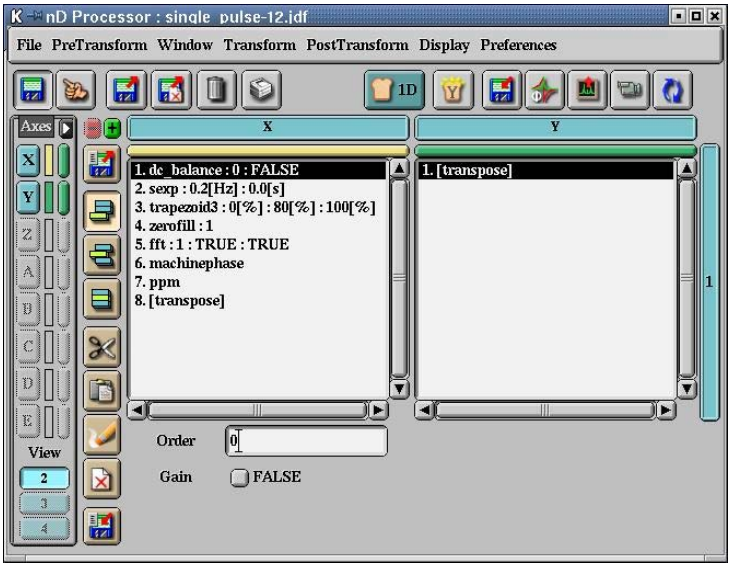
C I

4.2 PROCESSING METHOD FOR ARRAY MEASUREMENT DATA

4.2.1 Processing as a Single Data File

4.2.1a When process conditions are saved in the processing list

1. Load the desired processing list in the **nD Processor** window.

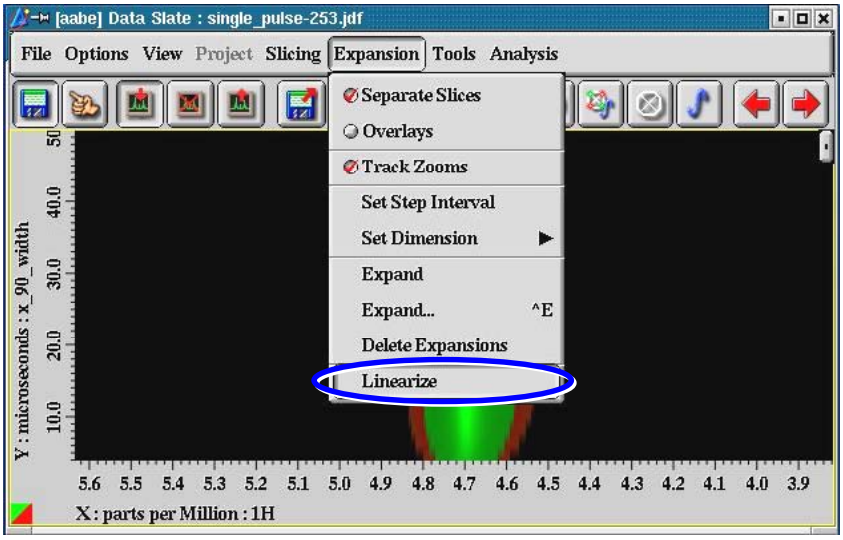


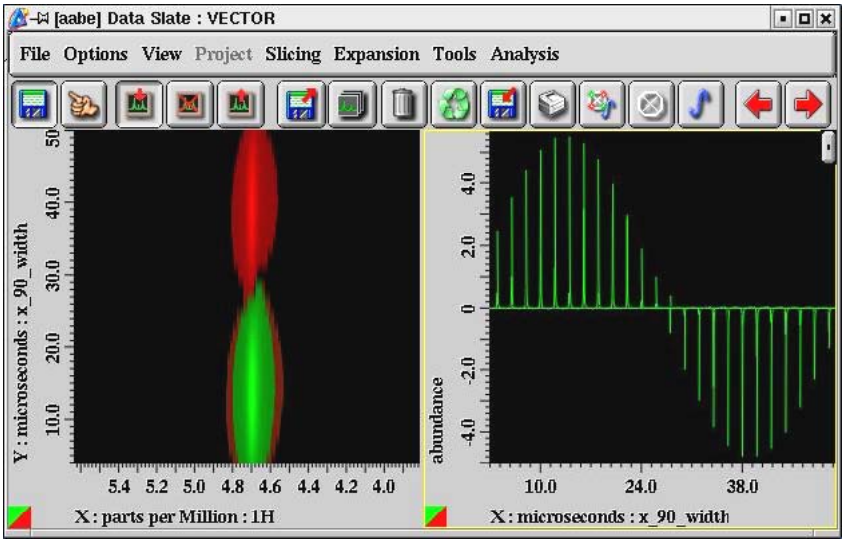
2. Click on the **Process File And Put In Data Slate** button.

After performing data processing specified by the process list for the first to the *n*th measurement data sets, the **Data Slate** window appears.

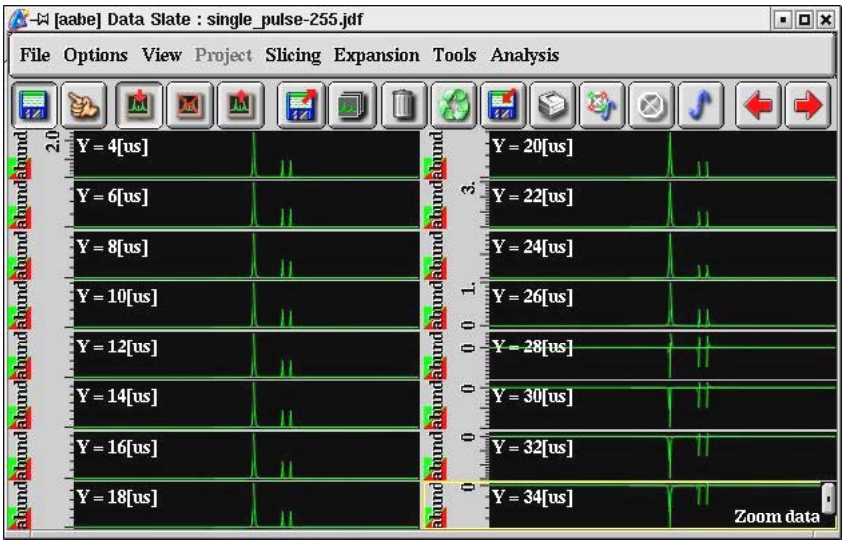
3. Select **Expansion-Linearize** from the menu bar in the **Data Slate** window.

One-dimensional data is displayed. It is used when specified signal intensity is observed (a 90° pulse, and decoupling map).




[aabe] Data Slate : VECTOR
File Options View Project Slicing Expansion Tools Analysis
Y : microseconds : x_90_width
X : parts per Million : 1H
abundance
X : microseconds : x_90_width

If you click on the **Will process data and put up to sixteen Y slices into Data Slate button** instead of the **Process File And Put In Data Slate** button, after performing data processing the process list for the first to nth measurement on data set, the processed data sets are displayed in the **Data Slate** window. The 1st to nth processed data sets are arranged in one window. These data sets are used to compare the details of each spectrum, such as in homonuclear spin decoupling and difference NOE.



Reference: A maximum of 16 processed data sets are displayed.
If n ≥ 17, a window opens, asking which processed data is to be displayed. 16 data are displayed from the specified position. All data can be displayed for 16 or fewer pieces.

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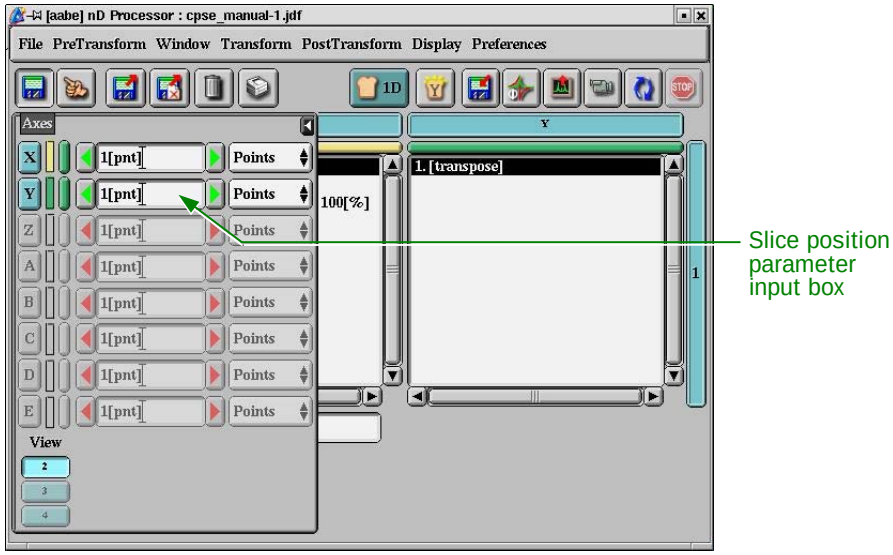
4.2.1b When the processing list is not provided

One data from the an array measurement data is displayed in the **1D Processor** window as one-dimensional slice data; suitable window function and phase correction values can be obtained using that data.

1. Click on the **X** button in the **nD Processor** window.

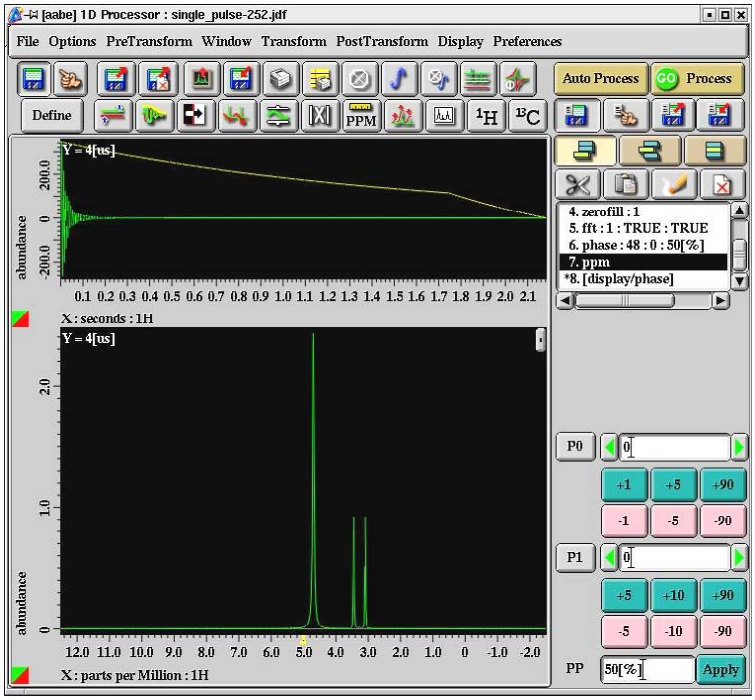
2. Enter the number (1 to n) of the slice data points in the slice position parameter input box.

Select data whose phase is easy to correct, and slice it.



3. Click on the 1D **1D Slice** button.

The slice data of the position specified in step 2 is displayed in the **1D Processor** window.



C I

4. Set an appropriate window function.

The operation is the same as changing the ordinary 1D data window function.

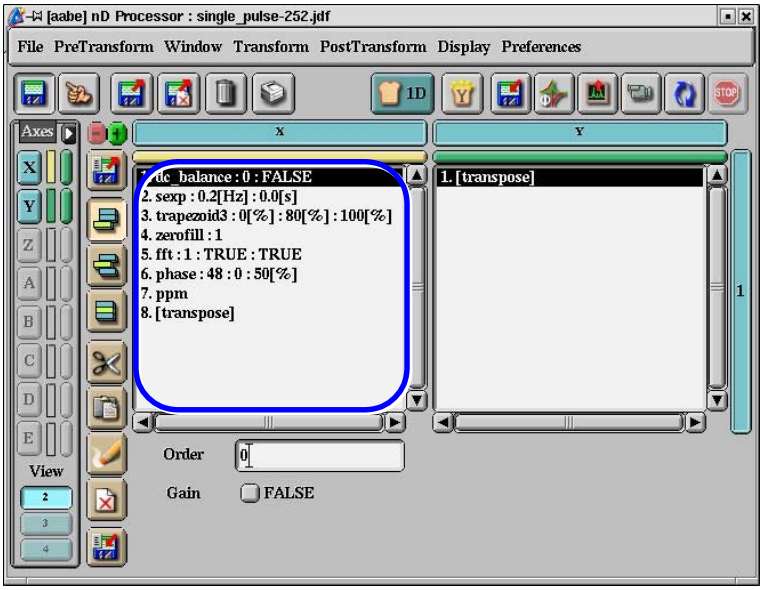
5. Perform the phase correction, to obtain an appropriate phase correction value.

The operation is the same as that performed the ordinary 1D data phase correction.

Be sure to perform manual not automatic phase correction.

6. Close the**1D Processor** window.

The window function and the phase correction values obtained in Steps 4 and 5 are automatically entered into the processing list in the **nD Processor** window.

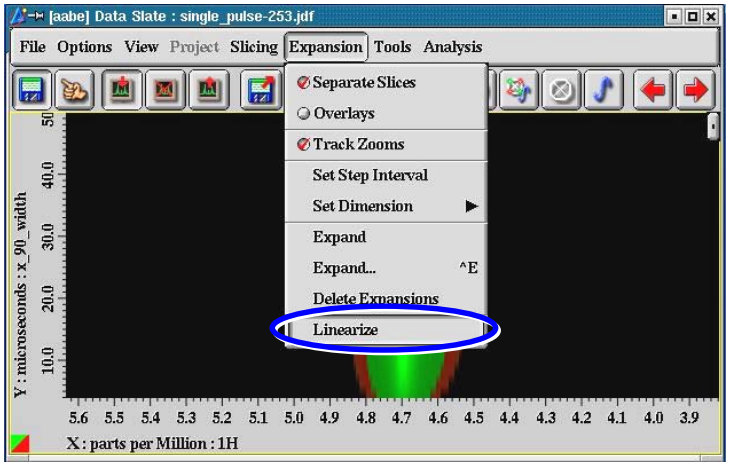


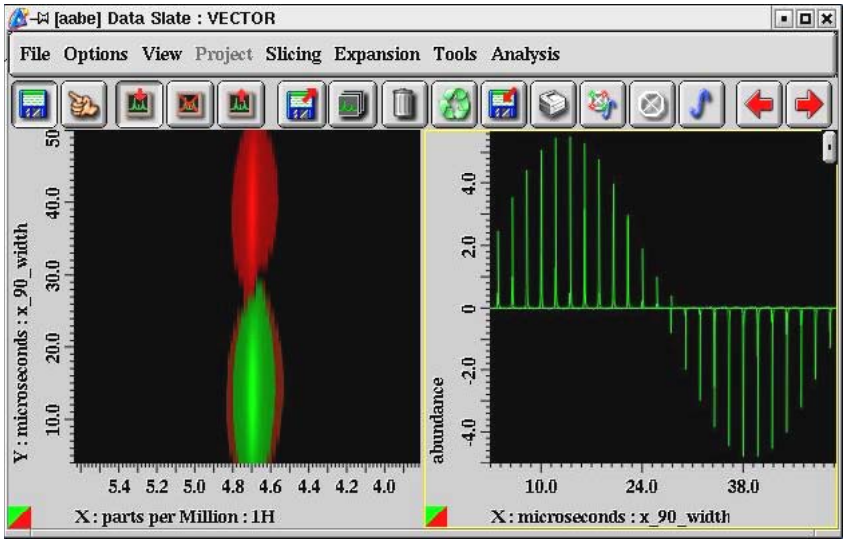
7. Click on the **Process File And Put In Data Slate** button.

After performing data processing of the processing list for the first to *n*th measurement data sets, the processed data sets are displayed in the **Data Slate** window.

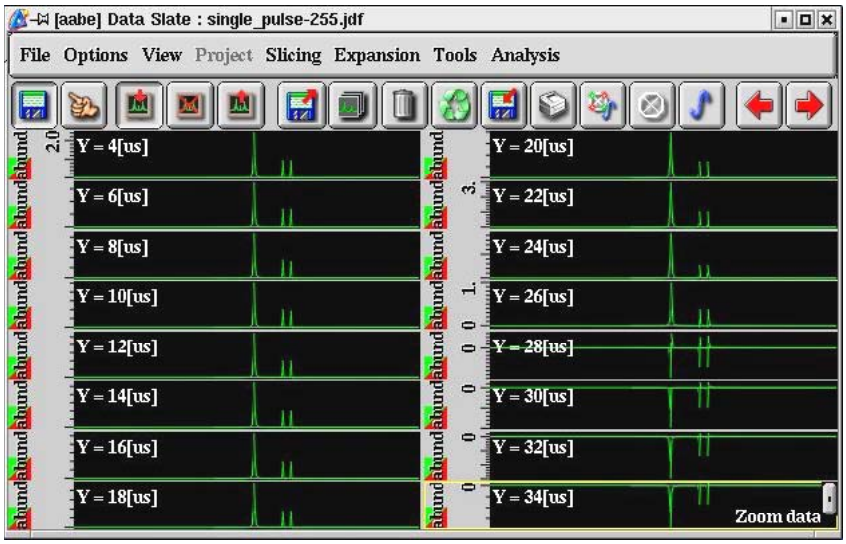
8. Select **Expansion-Linearize** from the menu bar in the **Data Slate** window.

1D data is displayed. This data is used to observe the change in intensity of the specific signal, such as in 90° pulse and decoupling map experiments.




[aabe] Data Slate : VECTOR
File Options View Project Slicing Expansion Tools Analysis
Y : microseconds : x_90_width
X : parts per Million : 1H
abundance
X : microseconds : x_90_width

If you click on the **Will process data and put up to sixteen Y slices into Data Slate button** instead of the **Process File And Put In Data Slate** button, after performing data processing of the process list for the first to nth measurement data set, the processed data sets are displayed in the **Data Slate** window. The 1st to nth processed data sets are arranged in one window. These data sets are used to compare the details of each spectrum, such as in homonuclear spin decoupling and difference NOE.



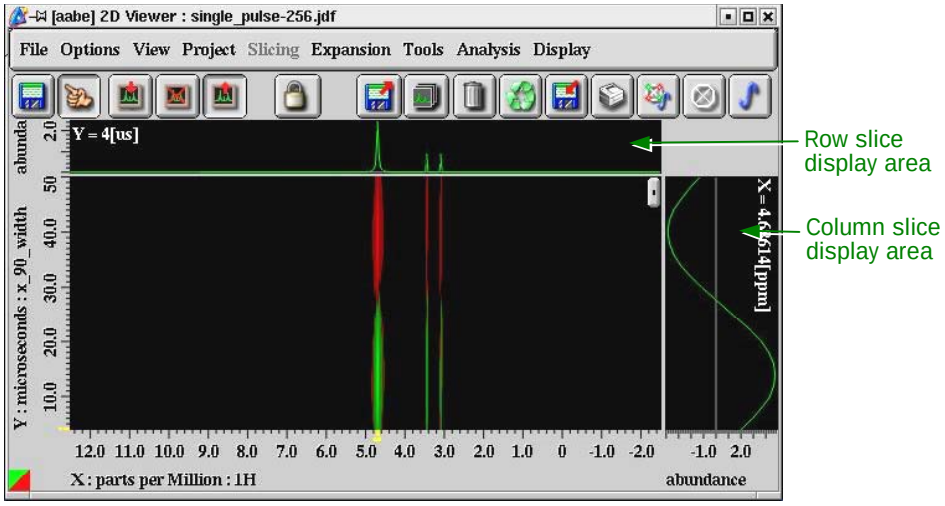
Reference: A maximum of 16 processed data sets are displayed.

If n ≥ 17, a window opens, asking which processed data is to be displayed. Only 16 data may be displayed from specified position. All data can be display when 16 or less data seta are displayed.

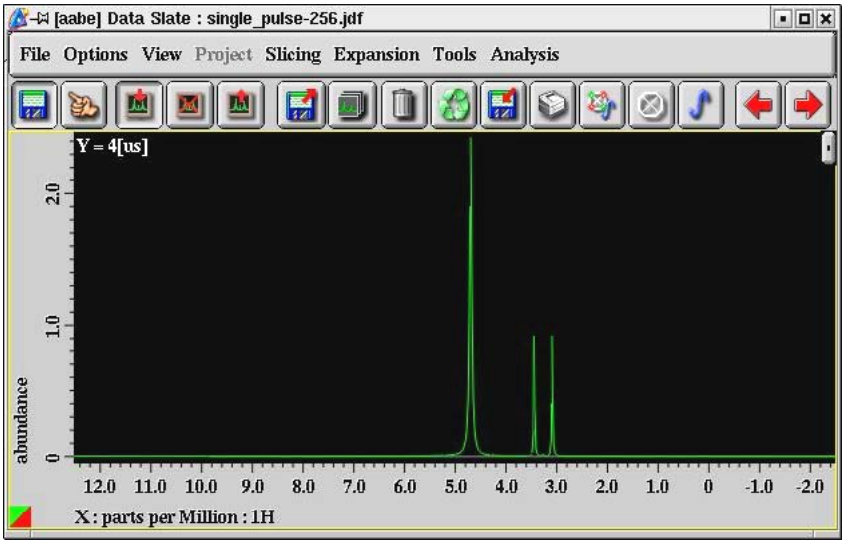
C I

4.2.1c Displaying data in the Data Slate window

1. Click on the **Process File And Put in Data Viewer** button after entering the process list in the **nD Processor** window.
2. Display the desired slice data in the row slice display area of the **Data Viewer** window.


[aabe] 2D Viewer : single_pulse-256.jdf
File Options View Project Slicing Expansion Tools Analysis Display
Y = 4[us]
Y : microseconds : x_90_width
X : parts per Million : 1H
abundance
Row slice display area
Column slice display area

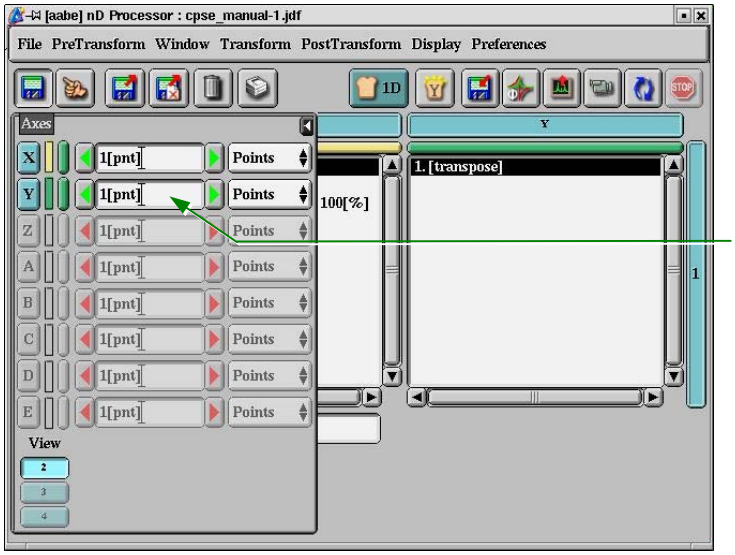
3. Click on the **Open Data By Fingering Geometry** button.
4. Click on the **Open Data to NEW Data Slate** button.
5. Click on the **Open Data File** button.
   The mouse pointer changes to the finger shape.
6. Move the mouse pointer to the row slice display area, and click on it.
   Slice data is displayed on the **Data Slate** window.


[aabe] Data Slate : single_pulse-256.jdf
File Options View Project Slicing Expansion Tools Analysis
Y = 4[us]
abundance
X : parts per Million : 1H

C I

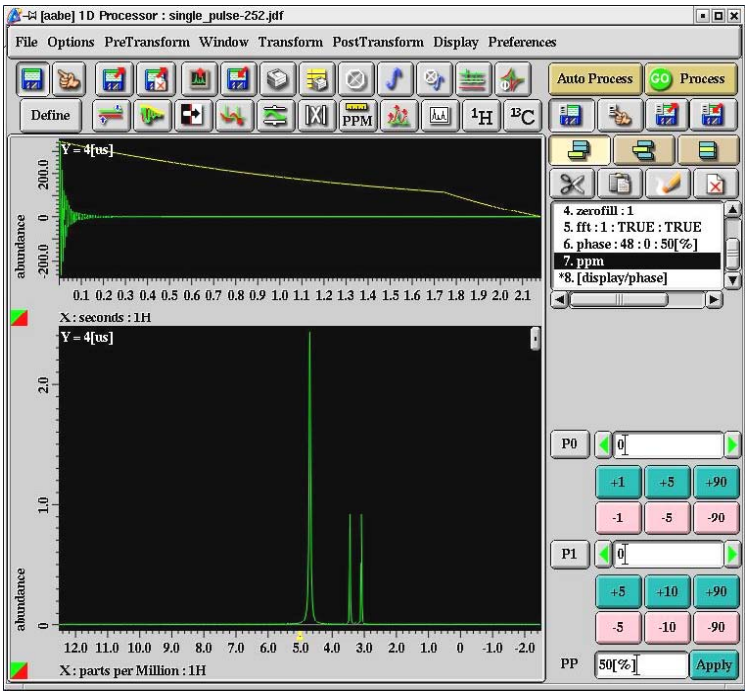
4.2.2 Processing Data taken from the Measurement Data Sets

1. Click on the **X** button in the **nD Processor** window.
2. Enter the position (the number of points) of the slice data to be processed into the Y-axis slice position parameter input box.



3. Click on the 1D **1D Slice** button.

   The slice data taken at the position specified in step 2 is displayed in the **1D Processor** window.



4. Perform data processing in the same way as ordinary 1D data processing.

If you want to save processed data after data processing is complete, save it in a file with a different name.

C I

5

ADDITION AND SUBTRACTION OF DATA

This chapter describes addition and subtraction of measurement data (FID) and processed data.
The **File Math** window is used for addition and subtraction of data.

5.1 **FILE MATH** WINDOW 5-1
5.2 ADDITION AND SUBTRACTION OF MEASUREMENT DATA (FID)..... 5-2
5.3 ADDITION AND SUBTRACTION OF PROCESSED DATA 5-4

C I

5.1 FILE MATH WINDOW

- Select **Tools**–**Math**–**File Math** from the **Delta Console** window.
  The **File Math** window opens.

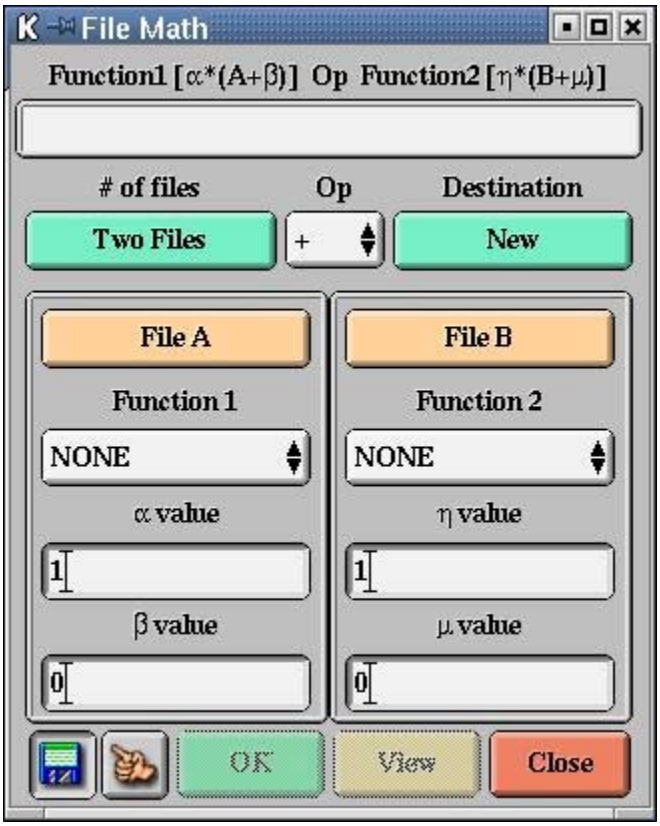


Fig. 5.1 File Math window

C I

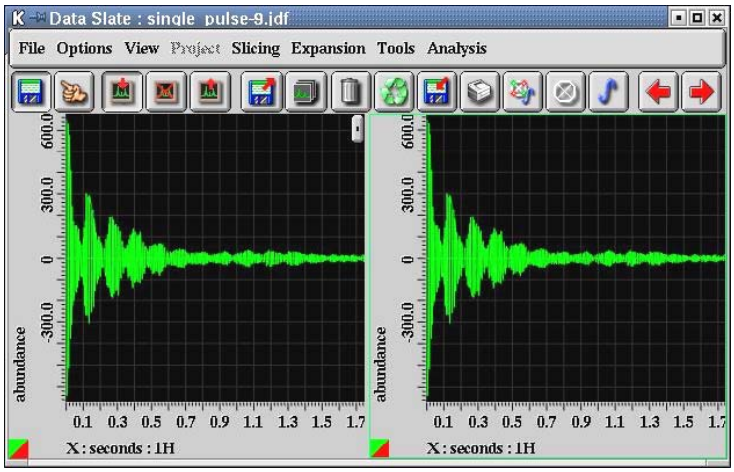
5.2 ADDITION AND SUBTRACTION OF MEASUREMENT DATA (FID)

The simple addition of measurement data (FID) is used, for example, to enhance the signal-to-noise ratio for more than one data set, which are measured under the same measurement conditions.

If the measurement temperatures are different because of long time intervals between measurements, or the sample concentrations are different because of quantities of solvents, the peak positions might be observed to be different between the data sets. In such a case, the peak becomes broad or multiple when measurement data (FID) are added, so that the S/N ratio is not enhanced.

■ To perform only addition of measurement data (FID)

1. Open the **File Math** window.
2. Display two measurement data sets (FID) for addition in the different geometries.



3. Click on the **# of files** selection button in the **File Math** window to display **Two Files**.

   Every time you click on the selection button, the display switches between **Two Files** and **One File**.

4. Select **+** by clicking on the **Op** selection buttons.
5. Click on the **Finger** button.
6. Click on the **File A** button.

   The mouse pointer changes to the shape of a finger.
7. Move the mouse pointer to one of the data display areas, and click on it.

   The filename of the data set you clicked on is displayed on the File A button.
8. Click on the **File B** button.

   The mouse pointer changes to the shape of a finger.

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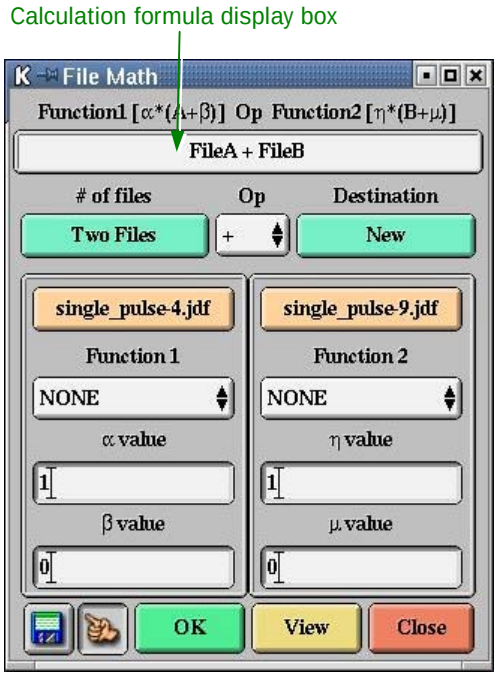
9. Move the mouse pointer to another data display area, and click on it.
The filename of the data set you clicked on is displayed on the **File B** button.

10. Select **NONE** using selection buttons **Function 1** and **Function 2**.

11. Enter 1 in both the **α value** and **η value** input boxes.

12. Enter 0 in both the **β value** and **μ value** input boxes.
The calculation formula **FileA+FileB** is displayed in the calculation equation display box.
Reference: The calculation **FileA+FileB** is simple addition.



13. Click on the **View** button.
The **Resulting File** window opens, and the calculated data is displayed.
Judge from the data whether or not the calculation formula is appropriate.

14. Click on the **View** button.
The **Resulting File** window closes.

15. Click on the **OK** button.
The calculated result is displayed in the **Data Slate** window.
The filename of the calculated result displayed in the **Data Slate** window is the same as on the **File A** button. Save it under a different filename, if necessary.
Reference: Then, the same data processing for normal 1D measurement data can be performed for the calculation result.

16. Click on the **Close** button.
The **File Math** window closes.

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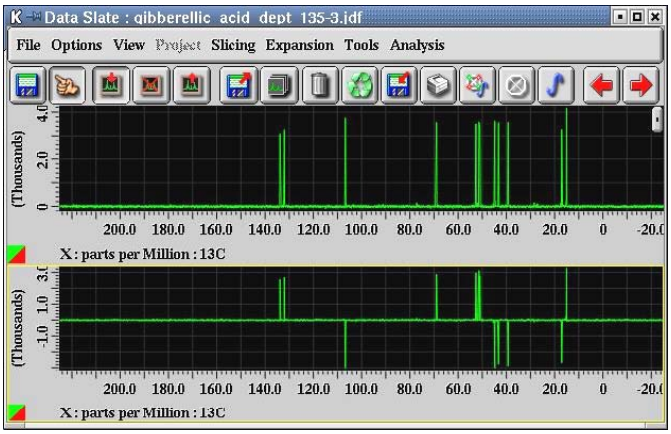
5.3 ADDITION AND SUBTRACTION OF PROCESSED DATA

■ To perform addition and subtraction of processed data

1. Open the **File Math** window.
2. Display two processed data sets for addition and subtraction in the different geometries.

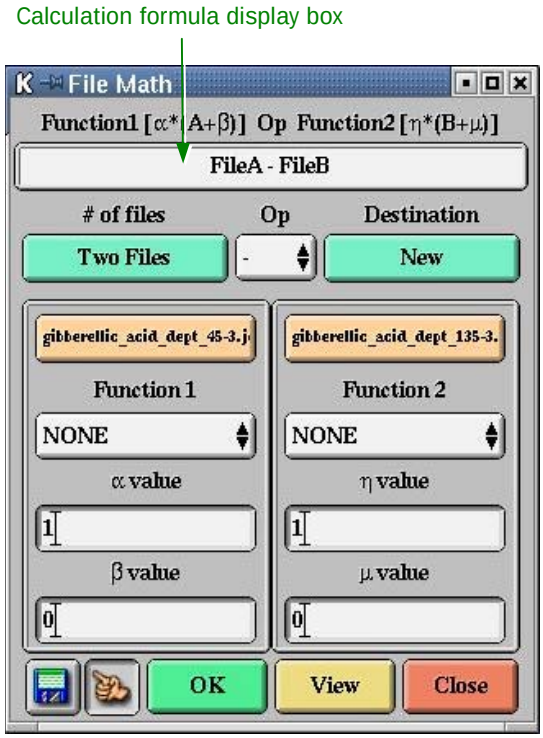

Data Slate : gibberellic acid dept 135-3.idf
File Options View Project Slicing Expansion Tools Analysis
(Thousands)
4.0
2.0
0
200.0 180.0 160.0 140.0 120.0 100.0 80.0 60.0 40.0 20.0 0
X : parts per Million : 13C
(Thousands)
3.0
1.0
-1.0
200.0 180.0 160.0 140.0 120.0 100.0 80.0 60.0 40.0 20.0 0
X : parts per Million : 13C

3. Click on the **# of files** selection button in the **File Math** window to display **Two Files**.
   Every time you click on the selection button, the display switches between **Two Files** and **One File**.

4. Select **+** or **–** by clicking on the **Op** arrow buttons.
5. Click on the **Finger** button.
6. Click on the **File A** button.
   The mouse pointer changes to the shape of a finger.
7. Move the mouse pointer to one of the data display areas, and click on it.
   The filename of the data set you clicked on is displayed on the **File A** button.
8. Click on the **File B** button.
   The mouse pointer changes to the shape of a finger.
9. Move the mouse pointer to another data display area, and click on it.
   The filename of the data set you clicked on is displayed on the **File B** button.
10. Select **NONE** using selection buttons **Function 1** and **Function 2**.
11. Enter **1** in the ***α* value** (intensity coefficient of **File A** data along the Y-axis) input box.
12. Enter **0** in the ***β* value** input box.
13. Enter an appropriate value in the ***η* value** (intensity coefficient of **File B** data along the Y-axis) input box.

14. Enter an appropriate value in the ***μ* value** input box.

The calculation formula with the coefficients that were set in Steps 10 to 14 is displayed in the calculation formula display box.



15. Click on the **View** button.

The **Resulting File** window opens, and the calculated data is displayed.
Judge from the data whether or not the calculation formula is appropriate.
If it is not appropriate, change the value in the ***η* value** or ***μ* value** input box.
Every time you change the value, calculation is automatically executed, and the calculated data is updated and displayed.

16. Click on the **View** button.

The **Resulting File** window closes.

17. Click on the **OK** button.

The calculated result is displayed in the **Data Slate** window.

The filename of the calculated result displayed in the **Data Slate** window is the same as on the **File A** button. Save it under a different filename, if necessary.

18. Click on the **Close** button.

The **File Math** window closes.

C I

DATA SLATE

The data slate is an all-purpose data display and analysis tool that can accept 1, 2, 3, or 4-dimensional data. While Data Viewer and Data Processor allows you to manipulate only one data set, Data Slate allows you to manipulate more than one data set in one window.

This data slate lets you easily overlap and connect data for comparison, analysis, and plotting.

6.1 DATA SLATE WINDOW 6-1
6.2 DISPLAYING DATA SLATE WINDOW 6-2
6.3 ADDITIONAL DISPLAY OF PROCESSED DATA 6-3
6.3.1 Displaying Additional Data in Another Geometry 6-4
6.3.2 Overlaying Additional Data in One Geometry 6-5
6.3.3 Display Control When Multiple Geometries are Displayed 6-7
6.3.4 Display Control for Multiple Data in a Geometry 6-11
6.4 PEAK PICK AND INTEGRATION 6-15

C I

6.1 DATA SLATE WINDOW

The **Data Slate** window is used to display multiple data sets for which data processing is complete. You can manipulate 1D and 2D data together.

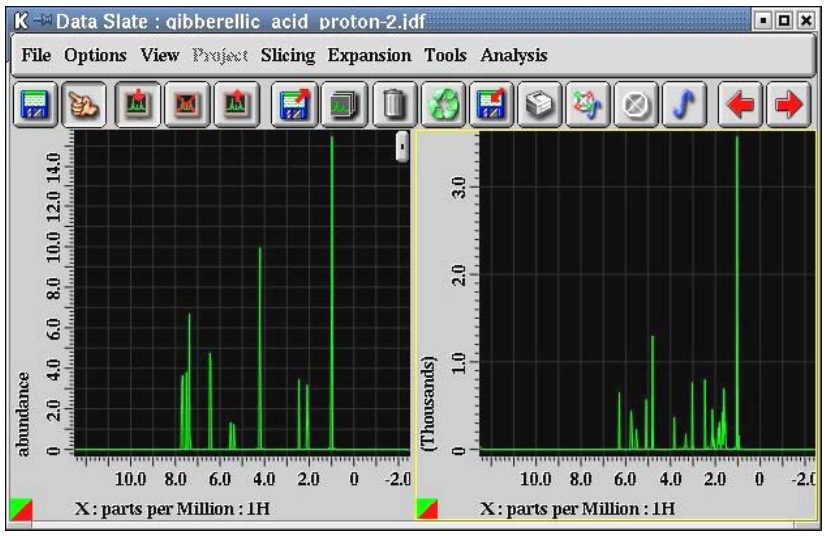

Data Slate : gibberellic_acid_proton-2.idf
File Options View Project Slicing Expansion Tools Analysis
abundance
(Thousands)
X : parts per Million : 1H
X : parts per Million : 1H

Fig. 6.1 Data display in the Data Slate window example 1

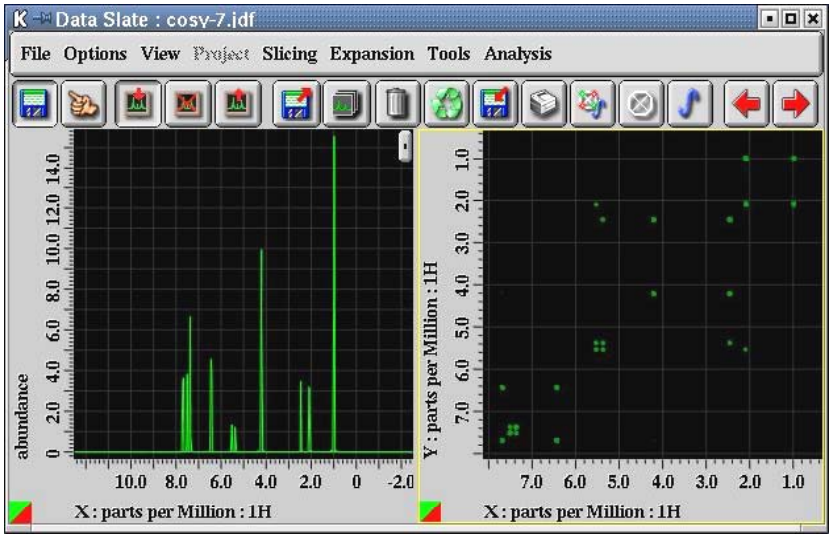
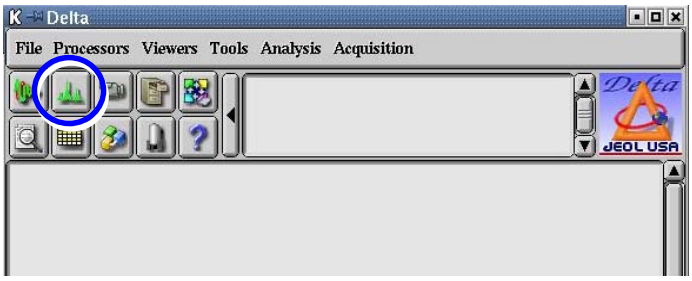

Data Slate : cosy-7.idf
File Options View Project Slicing Expansion Tools Analysis
abundance
Y : parts per Million : 1H
X : parts per Million : 1H
X : parts per Million : 1H

Fig. 6.2 Data display in the Data Slate window example 2

C I

6.2 DISPLAYING DATA SLATE WINDOW

1. Click on the **Data Slate** button in the **Delta Console** window.



The **Open Data for Data Slate** window opens.

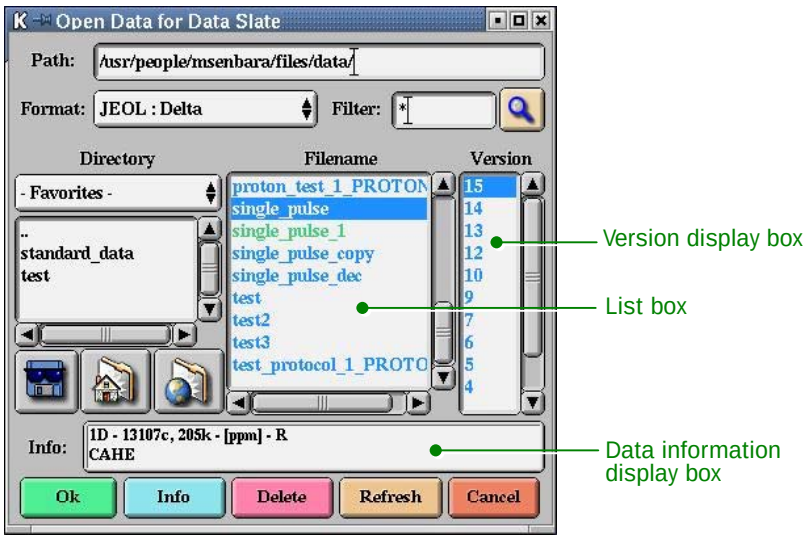


Fig. 6.3 Open Data for Data Slate window

2. Verify the contents of the data information display box from the list box, and select the data file you want to read in and its version.

3. Click on the **Ok** button.

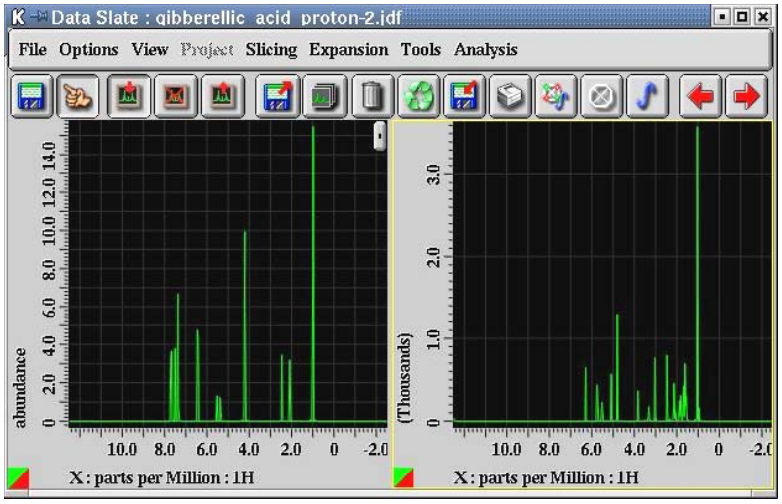
The processed data (Fourier transformed data) is displayed in the **Data Slate** window.

C I

6.3 ADDITIONAL DISPLAY OF PROCESSED DATA

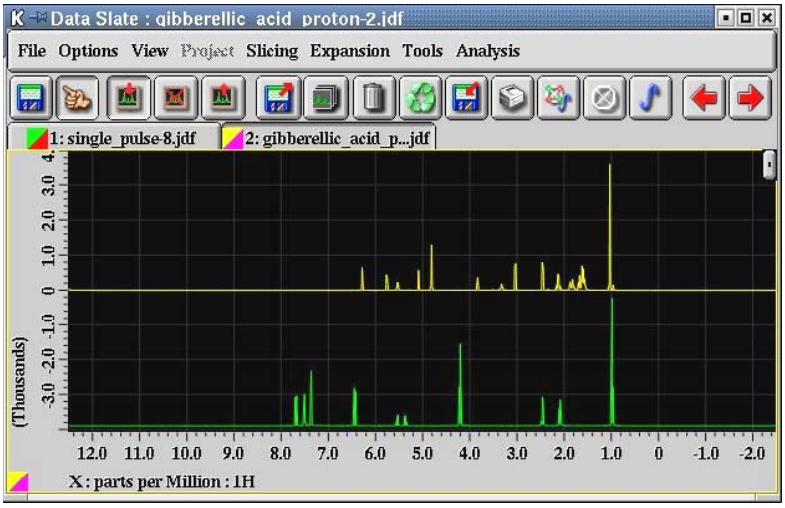
There are the following two ways for additional display.

- Displaying additional data in another geometry


Data Slate : gibberellic_acid_proton-2.jdf
File Options View Project Slicing Expansion Tools Analysis
abundance
(Thousands)
X : parts per Million : 1H
X : parts per Million : 1H

Reference: A geometry is a process data display area. The above **Data Slate** window consists of two geometries.

- Overlaying additional data in one geometry.


Data Slate : gibberellic_acid_proton-2.jdf
File Options View Project Slicing Expansion Tools Analysis
1: single_pulse-8.jdf
2: gibberellic_acid_p...jdf
(Thousands)
X : parts per Million : 1H

C I

6.3.1 Displaying Additional Data in Another Geometry

■ If the additional data is saved on a disk

1. Click on the **Open Data From Disk** button in the **Data Slate** window.
2. Click on the **Open Data to This Tool** button.
3. Click on the **Open Data File** button.
   The **Open File** window opens.

Fig. 6.4 Open File window

4. Select the data file that you want to display in addition from the list box in the **Open File** window, and click on the **Ok** button.
   The data saved in the selected file is displayed in another geometry.

■ If the additional data is being displayed

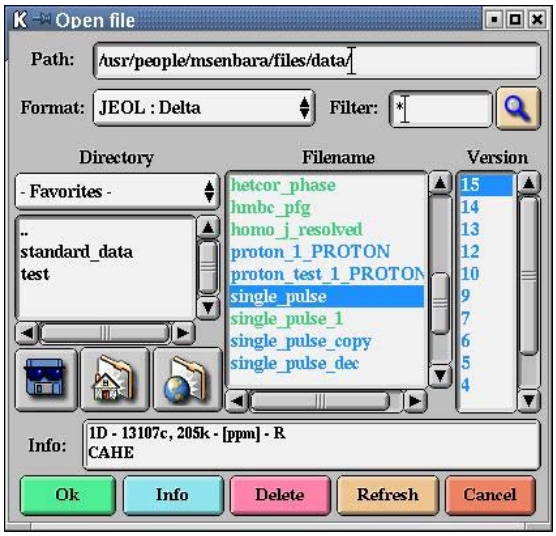
1. Click on the **Open Data By Fingering Geometry** button in the **Data Slate** window.
2. Click on the **Open Data to This Tool** button.
3. Click on the **Open Data File** button.
   The mouse pointer changes to the shape of a finger.
4. Move the mouse pointer to the area in which the additional data is displayed, and click on it.
   The data you clicked on is displayed in another geometry.

C I

6.3.2 Overlaying Additional Data in One Geometry

■ If the additional data is saved on a disk

1. Select the **Select** mode from the cursor tool bar in the process data display area in the **Data Slate** window.
2. Click on the **Select geometry** button in the **Select** mode.
3. Move the mouse pointer into the geometry in which you want to display additional data, and click on it.
   The color of the mouse pointer changes to yellow.
4. Click on the **Open Data From Disk** button.
5. Click on the **Open Data to This Tool** button.
6. Click on the **Open Data as Overlay on Currently Selected Geometry** button.
   The **Open File** window opens.



7. Select the additional data file that you want to display from the list box in the **Open File** window, and Click on the **Ok** button.
   The data saved in the selected file is displayed in addition in the geometry selected in Step 3.

The additional data is overlaid on the first displayed data in a different color.
If you wish, you can change the display position, following the procedure of Section 6.3.4.

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If the additional data is being displayed

1. Select the **Select** mode from the cursor tool bar menu in the process data display area in the **Data Slate** window.
2. Click on the **Select geometry** button in the **Select** mode.
3. Move the mouse pointer into the geometry in which you want to display additional data, and click on it.
   The color of the mouse pointer changes to yellow.
4. Click on the **Open Data By Fingering Geometry** button.
5. Click on the **Open Data to This Tool** button.
6. Click on the **Open Data as Overlay on Currently Selected Geometry** button.
   The mouse pointer changes to the shape of a finger.
7. Move the mouse pointer to the area in which the additional data is displayed, and click on it.
   The data you clicked on is displayed in the geometry selected in Step 3.

The additional data is overlaid on the first displayed data.
If you wish, you can change the display position, following the procedure of Section 6.3.4.

C I

6.3.3 Display Control When Multiple Geometries are Displayed

To align all geometries vertically

- Select **View**–**Horizontal** in the **Data Slate** window.
  The geometries are aligned vertically.

To align all geometries horizontally

- Select **View**–**Vertical** in the **Data Slate** window.
  The geometries are aligned horizontally.

To switch the displays of two geometries

1. Select **View**–**Swap** in the **Data Slate** window.
   The mouse pointer changes to the shape of a finger.
2. Move the mouse pointer to one geometry in which you want to change the display, and click on it.
   The mouse pointer returns to the shape of the arrow.
3. Move the mouse pointer to another geometry, and click on it.
   The displays of the two geometries selected in Steps 2 and 3 will be switched.

The above operation is in effect only between two geometries in the same **Data Slate** window. You cannot swap the geometries in different **Data Slate** windows.

To delete a geometry

1. Select the **Select** mode from the cursor tool bar.
2. Click on the **Select geometry** button in the **Select** mode.
3. Move the mouse pointer to the geometry you want to delete, and click on it.
   The mouse pointer changes to yellow (showing the display selected).
4. Click on the **Close Currently Selected Geometry** button.
   The geometry selected in Step 3 will be deleted.

To display a geometry in another new *Data Slate* window

1. Click on the **Open Data By Fingering Geometry** button.
2. Click on the **Open Data to New Data Slate** button.
3. Click on the **Open Data File** button.
   The mouse pointer changes to the shape of a finger.
4. Move the mouse pointer to the geometry in another new **Data Slate** window, and click on it.
   The selected geometry will be displayed in another new **Data Slate** window.

C I

To make the horizontal scale the same in all geometries displayed in one Data Slate window

1. Select **View–Connect X** in the **Data Slate** window.
   The **Connect X** button is checked.
2. Expand data in any geometry horizontally.
   The horizontal scale in the other geometries follows.
   The vertical size does not change.

To make the horizontal and vertical scales the same in all geometries displayed in one Data Slate window

1. Select **View–Connect All** in the **Data Slate** window.
   The **Connect All** button is checked.
2. Expand data in any geometry.
   The horizontal and vertical scales for the other geometries follows.

Connecting two geometries to set the expansion range to the same value

The following operation takes effect between two geometries displayed in the same **Data Slate** window or in different **Data Slate** windows.

1. Select **Tools–Connection Tool** in the **Data Slate** window.
   The **Connection Tool** window opens.

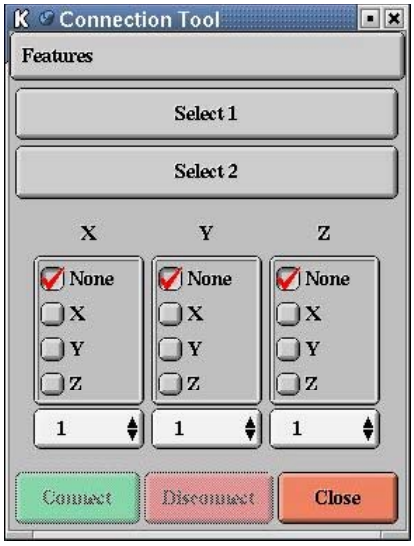


Fig. 6.5 Connection Tool window

2. Select **Features–Zoom** in the **Connection Tool** window.
   The **Zoom** button is checked.

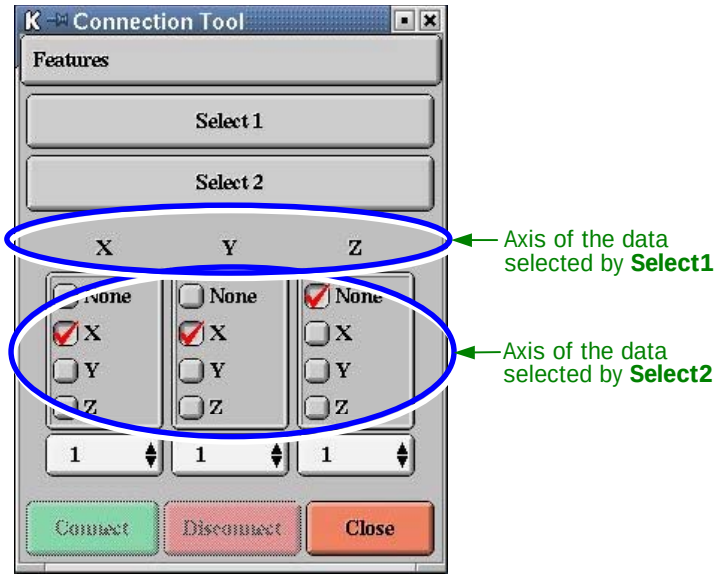
   If the **Zoom** button had already been checked, you can omit the following Step 3.
3. Click on the **Select1** button.
   The mouse pointer changes to the shape of a finger.

4. Move the mouse pointer to the geometry in which you want to expand the data to the same range, and click on it.
The file name is displayed on the **Select1** button.

5. Click on the **Select2** button.
The mouse pointer changes to the shape of a finger.

6. Move the mouse pointer to the other geometry in which you want to expand the data to the same range, and click on it.
The file name is displayed on the **Select2** button.
Reference: You can select the geometry displayed in a different **Data Slate** window in this step.

7. Check the buttons of the axes of the data selected by **Select2** to be connected with those of the data selected by **Select1** by clicking on them respectively.



For example, to expand the horizontal and vertical axes of both the 1D data sets to the same size, check the **Select2 X-**axis button corresponding to the **Select1 X-**axis, and check the **Select2 Y-**axis button corresponding to the **Select1 Y-**axis as shown in the above figure.
Reference: You can make a connection between a 1D data geometry and a 2D data geometry.

8. Click on the **Connect** button.
The color of the **Select1** and **Select2** buttons changes, and the two geometries are connected.

9. Expand the **Select1** data or the **Select2** data.
The axes selected in Step 7 of the **Select1** and **Select2** data sets are expanded in the same ranges.

10. Click on the **Close** button.
The **Connection Tool** window closes.

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■ Disconnecting two connected geometries

1. Select **Tools**–**Connection Tool** in the **Data Slate** window.
   The **Connection Tool** window opens.
2. Click on the **Select1**button.
   The mouse pointer changes to the shape of a finger.
3. Move the mouse pointer to one of the geometries which you want to disconnect, and click on it.
   A file name is displayed on the **Select1** button.
4. Click on the **Select2** button.
   The mouse pointer changes to the shape of a finger.
5. Move the mouse pointer to the other geometry you want to disconnect, and click on it.
   A file name is displayed on the **Select2** button.
6. Click on the **Disconnect** button.
   The file names on the **Select1** button and **Select2** button disappear and the geometries will be disconnected.
7. Click on the **Close** button.
   The **Connection Tool** window closes.

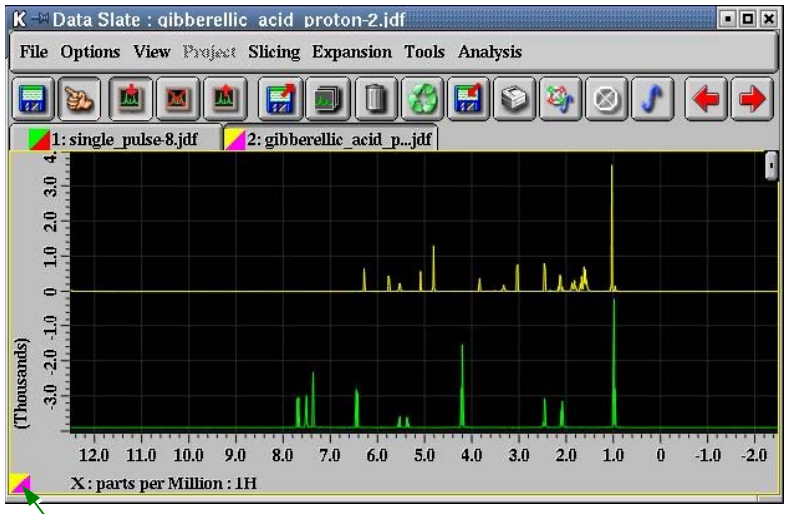
■ Setting two 2D data contour lines to the same level

1. Select two data connected according to the above procedure, "■Connecting two geometries to expand the data to the same range".
2. Select **Contour** from the **Features** menu in the **Connection Tool** window.
3. Click on the **Connection** button.
4. Recalculate the contour lines for one of the 2D data sets using the **Apply** button in the **Level Tool** window.
   The same setting of the contour lines will automatically be done for both sets of the 2D data.

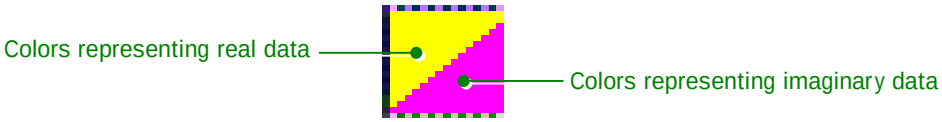
6.3.4 Display Control for Multiple Data in a Geometry

■ Displaying multiple data overlaid in one geometry

The first data is displayed in green. The data added next is displayed in yellow. The next data is displayed in orange. When additional multiple data sets are displayed in one geometry, each data is displayed in a different color. The color of the selection data display box also changes to the display color of the currently selected data.


Data Slate : gibberellic_acid_proton-2.jdf
File Options View Project Slicing Expansion Tools Analysis
1: single_pulse-8.jdf
2: gibberellic_acid_p...jdf
(Thousands)
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0 -1.0 -2.0
X : parts per Million : 1H
Selection data display box

For example, if the second added data is selected, the colors of the selection data display box become yellow for the real data and pink for the imaginary data.



The scale (X Ruler and Y Ruler) display changes to the scales corresponding to the currently selected data.

■ Changing the selected data

1. Select the **Offset** mode from the cursor tool bar in the process data display area in the **Data Slate** window.
2. Click on the **Cycle overlays** button in the **Offset** mode.
3. Move the mouse pointer to the process data display area, and click on it.
   The color of the selection data display box changes. Every time you click on it, the color of the selection data display box changes.
   The color of the selection data display box represents the display color of the currently selected data.

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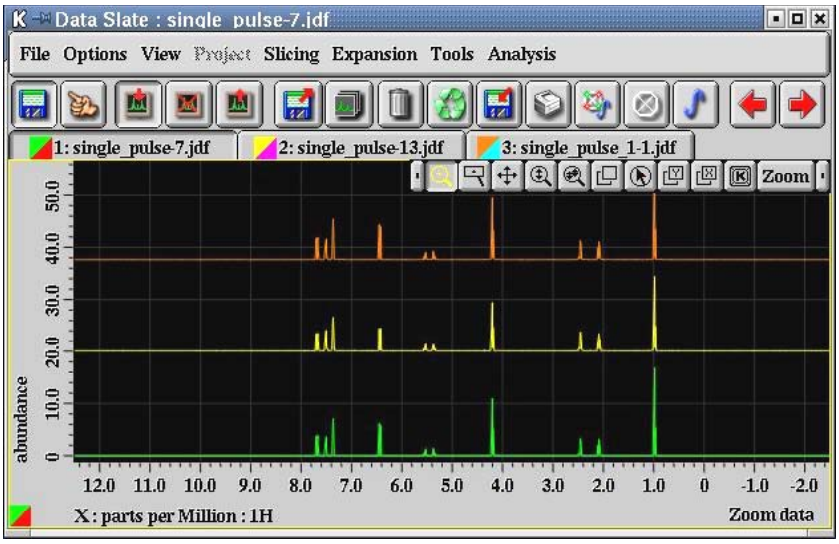
■ Changing the display position of the selected data along the Y axis

1. Select the data whose display position you want to change along the Y axis according to the above procedure, "■Changing the selected data".
2. Select the **Zoom** mode from the cursor tool bar in the process data display area.
3. Click on the **Offset overlay in Y** button in the **Zoom** mode.
4. Move the mouse pointer to the process data display area, and press and hold the left mouse button.
   The display position setting cursor is displayed.
5. Move the mouse pointer with the mouse button pressed to the display position along the Y axis, and release it.
   The display position of the data selected in Step 1 changes along the Y axis.

✍ The display position of the data displayed first in the **Data Slate** window cannot be changed.



■ Changing the display position of the selected data along the X axis

1. Select the data whose display position you want to change along the X axis according to the above procedure, "■Changing the selected data".
2. Select the **Zoom** mode from the cursor tool bar in the process data display area.
3. Click on the **Offset overlay in X** button in the **Zoom** mode.
4. Move the mouse pointer to the process data display area, and press and hold the left mouse button.
   The display position setting cursor is displayed.
5. Move the mouse pointer with the mouse button pressed to the display position along the X axis, and release it.
   The display position of the data selected in Step 1 changes along the X axis.

✍ The display position of the data displayed first in the ***Data Slate*** window can not be changed.

■ Changing the display position of the selected data along the X and Y axes

1. Select the data whose display position you want to change along the X and Y axes according to the above procedure, "■Changing the selected data".
2. Select the **Zoom** mode from the cursor tool bar in the process data display area.
3. Click on the **Offset overlay in X** button in the **Zoom** mode.
4. Move the mouse pointer to the process data display area, and press and hold the left mouse button.
   The display position setting cursor is displayed.
5. Move the mouse pointer with the mouse button pressed to the display position along the X and Y axes, and release it.
   The display position of the data selected in Step 1 changes along the X and Y axes.

✍ The display position of the data displayed first in the **Data Slate** window cannot be changed.

■ Returning the display position of all data to the initial state (the same display position as when first displayed)

1. Select the **Zoom** mode from the cursor tool bar in the process data display area.
2. Move the mouse pointer to the button (key command display button), and press and hold the left mouse button.
   The key commands are displayed.
3. Move the mouse pointer to **Recenter All A** with the mouse button pressed, and release it.
   The display position of all data returns to the initial state.

■ Returning the display position of the selected data to the initial state (the same display position as when first displayed)

1. Select the data whose display position you want to return to the initial state according to the above procedure, "■Changing the selected data".
2. Select the **Zoom** mode from the cursor tool bar in the process data display area.
3. Move the mouse pointer to the button, and press and hold the left mouse button.
   The key commands are displayed.
4. Move the mouse pointer to **Recenter [R]** with the mouse button pressed, and release it.
   The display position of the data selected in Step 1 returns to the initial state.

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■ Deleting the selected data

1. Select the **Select** mode from the cursor tool bar in the process data display area in the **Data Slate** window.
2. Click on the **Select geometry** button in the **Select** mode.
3. Move the mouse pointer to the geometry in which the data you want to delete is displayed, and click on it.
   The color of the mouse pointer changes to yellow, indicating the selection.
4. Select the data you want to delete according to the procedure, "■Changing the selected data".
5. Click on the **Remove Selected Overlay Data from Selected Geometry** button.
   The data, which was selected in Step 4, is deleted.

C I

6.4 PEAK PICK AND INTEGRATION

When data is loaded into the **Data Slate** window, peak information is also loaded.
For example, if the data is loaded in the **Data Slate** window after peak pick or integration is executed in the **1D Processor** window, peak information or integration can be displayed with the corresponding display option on.
Peak pick and integration (automatic and manual) can be performed in the **Data Slate** window in the same way as in the **1D Processor** window.
The **Data Slate** window can be used to perform peak pick and integration (automatic and manual) in the same way as the **1D Processor** window.

Curve fitting

When data is loaded into the **Data Slate** window, all information on curve fitting is also loaded together. Then, if the curve fitting has already been carried out in the **1D Processor** window, simply turning on the display option by selecting **Options**–**Peak** –**Peak Deconvolve** from the mouse right button menu displays the result.

Comment

A comment is also saved together with data.
Merely turning the display option on by selecting **Options**–**Annotation** from the mouse right button menu displays the result.
The comment can be put on data in the **Data Slate** window in the same way as in the **1D Processor** window.

Spread sheet tool

The spread sheet tool is used to display or print information on data, such as peaks, integration and attributes.
The spread sheet tool can be used in the **Data Slate** window in the same way as in the **1D Processor** window.

Printing data

The **print** button can be used in the **Data Slate** window in the same way as in the **1D Processor** window.

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7

SPREAD SHEET

The spread sheet tool is used to display or print information on data, such as peaks, integration and attributes.

7.1 SPREAD SHEET WINDOW 7-1
7.2 DISPLAYING THE RESULTS OF PEAK PICK AND INTEGRATION 7-2
7.3 PRINTING TABLES 7-5
7.4 STORAGE USING ASCII FILE 7-6

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7.1 SPREAD SHEET WINDOW

The detailed results of peak pick and integration are displayed in the form of tables in the **Spread Sheet** window as shown below.

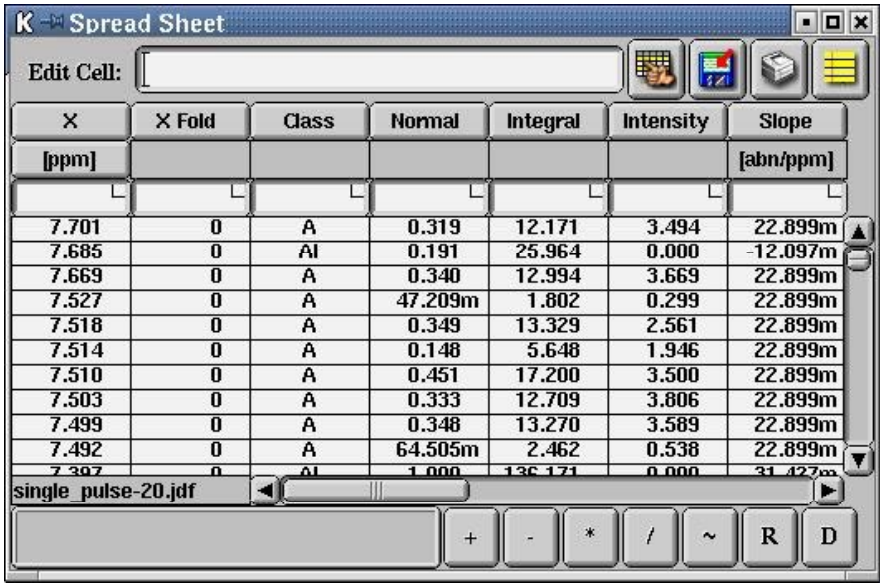

Fig. 7.1 Spread Sheet window

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7.2 DISPLAYING THE RESULTS OF PEAK PICK AND INTEGRATION

To display results

1. Click on the **Spread Sheet** button in the **Delta Console** window.
   The **Spread Sheet** window opens.
2. Click on the **Finger Data in Geometry** button in the **Spread Sheet** window.
   The mouse pointer changes to the shape of the finger.
3. Move the mouse pointer to the spectral area in which the data used for obtaining the results of peak pick and integration is displayed, and click on it.
   The detailed results of peak pick and integration are displayed in the **Spread Sheet** window.

To distinguish between the results of peak pick and integration

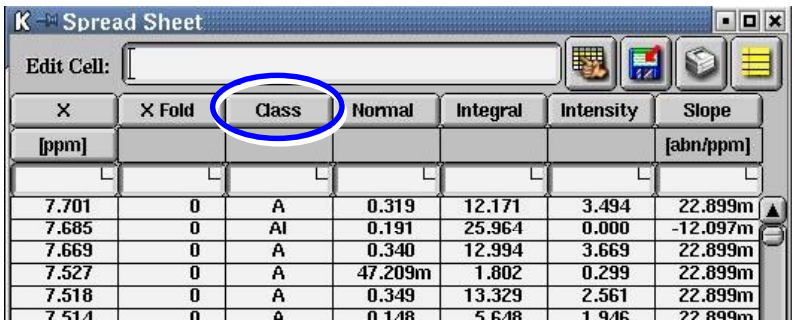
If you carry out peak pick and integration, the results of peak pick and integration are displayed in the order of ppm in the **Spread Sheet** window.
The results of peak pick and integration can be distinguished alphabetically in **Class** as show in the following table.

Table 7.1 Meaning of code in Class

	Result
A	Automatic peak pick
M	Manual peak pick
AI	Automatic integration
MI	Manual integration
SX	Peak pick selected currently (X=A, M), or integration result (X=AI, MI)
D	Currently selected integration

To distinguish between the results of peak pick and integration on a mixed display

- Click on the **Class** button in the **Spread Sheet** window.



The display changes to the alphabetical order in **Class**.

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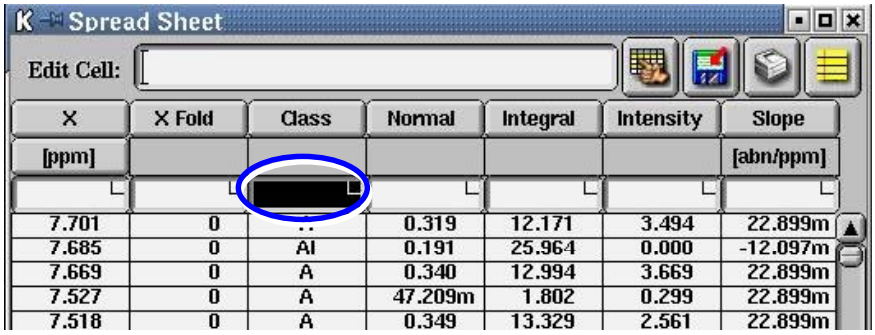
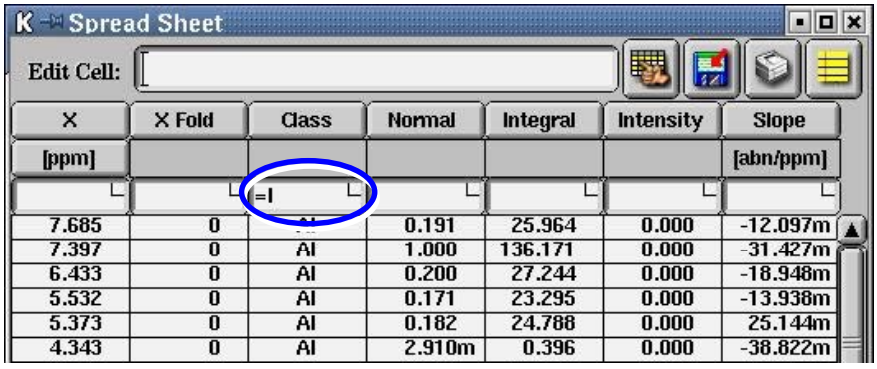
To display only the results of integrations from the results of peak pick and integrations

1. Click on the blank cell under the **Class** button in the **Spread Sheet** window.
   The clicked cell becomes highlighted.

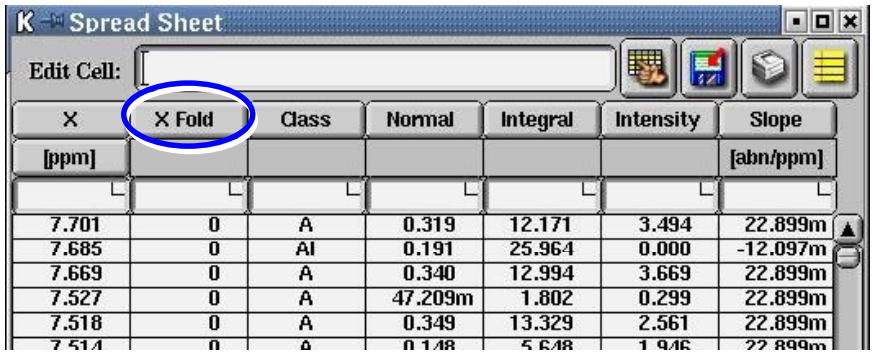


2. Enter "=I" from the keyboard.
   Only the results of integrations are displayed.



To delete the selected columns

1. Move the mouse pointer onto the item you want to delete in the **Spread Sheet** window.



2. Press the middle mouse button.
   The selected columns are deleted.

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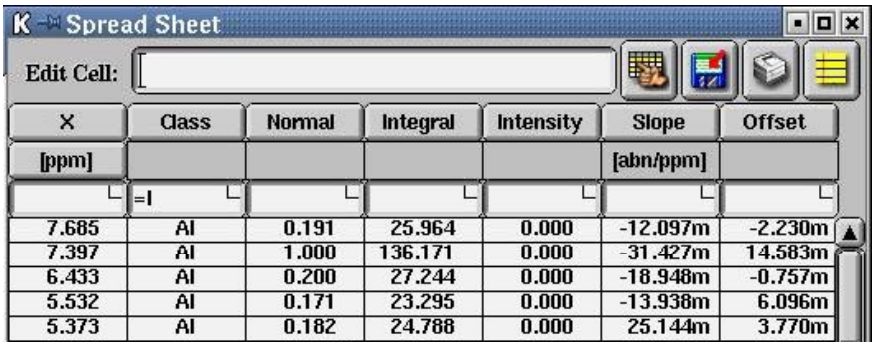
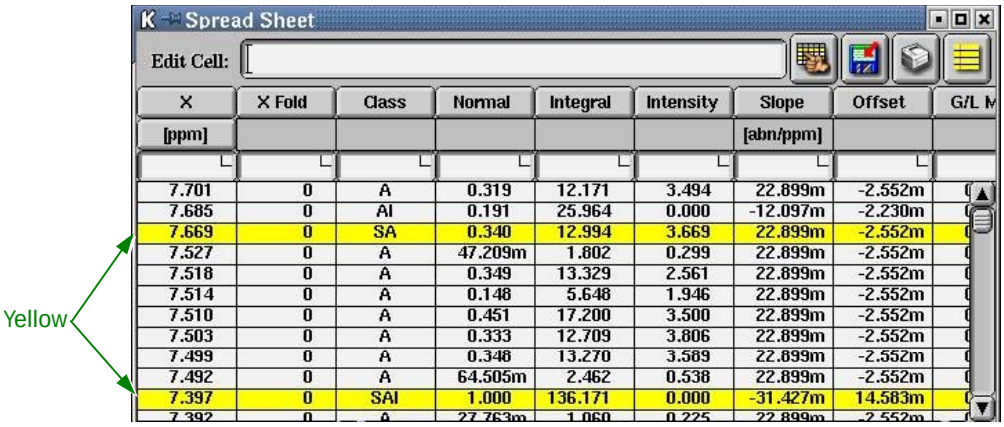


X [ppm]	Class	Normal	Integral	Intensity	Slope [abn/ppm]	Offset
	=I					
7.685	AI	0.191	25.964	0.000	-12.097m	-2.230m
7.397	AI	1.000	136.171	0.000	-31.427m	14.583m
6.433	AI	0.200	27.244	0.000	-18.948m	-0.757m
5.532	AI	0.171	23.295	0.000	-13.938m	6.096m
5.373	AI	0.182	24.788	0.000	25.144m	3.770m

■ Displaying the currently selected peak pick and integration

The letter “S” is displayed in **Class** and the lines for the currently selected peak pick and integration are displayed in yellow.



X [ppm]	X Fold	Class	Normal	Integral	Intensity	Slope [abn/ppm]	Offset	G/L M
7.701	0	A	0.319	12.171	3.494	22.899m	-2.552m	
7.685	0	AI	0.191	25.964	0.000	-12.097m	-2.230m	
7.669	0	SA	0.340	12.994	3.669	22.899m	-2.552m	
7.527	0	A	47.209m	1.802	0.299	22.899m	-2.552m	
7.518	0	A	0.349	13.329	2.561	22.899m	-2.552m	
7.514	0	A	0.148	5.648	1.946	22.899m	-2.552m	
7.510	0	A	0.451	17.200	3.500	22.899m	-2.552m	
7.503	0	A	0.333	12.709	3.806	22.899m	-2.552m	
7.499	0	A	0.348	13.270	3.589	22.899m	-2.552m	
7.492	0	A	64.505m	2.462	0.538	22.899m	-2.552m	
7.397	0	SAI	1.000	136.171	0.000	-31.427m	14.583m	
7.392	0	A	27.763m	1.060	0.225	22.899m	-2.552m	

In the above example, two lines are displayed in yellow, showing that two integration curves are selected at present.

7.3 PRINTING TABLES

- Click on the **Plot Spread Sheet** button of the **Spread Sheet** window.
  The table is printed.

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7.4 STORAGE USING ASCII FILE

1. Click on the **Save Spread Sheet in ASCII** button of the **Spread Sheet** window.

The **Save File** window opens.

2. Enter the filename into the filename input box in the **Save File** window.

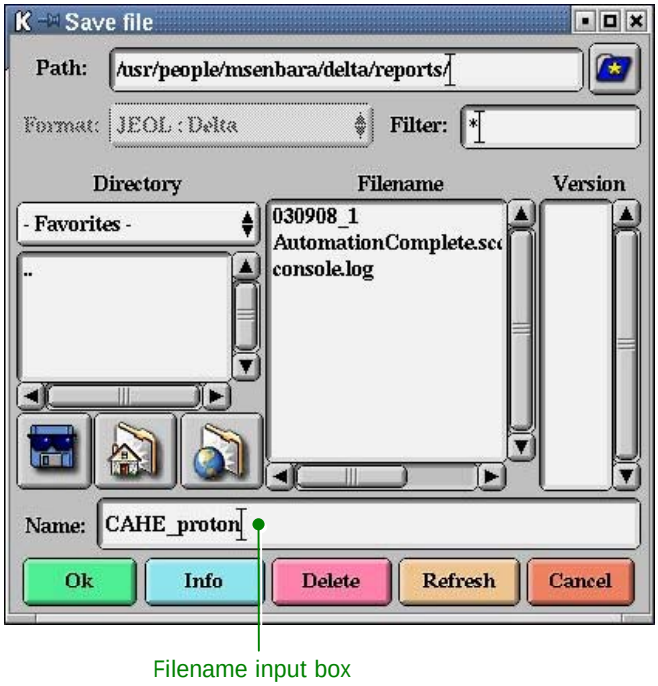

Fig. 7.2 Save File window

When creating a new directory, after specifying a directory name in the **Path** input box, click on the button. Create the directory and move it. After that, enter the filename to save it into the filename entry box.

3. Click on the **Ok** button.

The table in the **Spread Sheet** window is saved under the filename specified in Step 2.

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TREATMENT OF 3D DATA

8.1 DISPLAY OF 3D DATA 8-1
8.1.1 **3D Viewer** Window 8-1
8.1.2 **Data Slate** Window 8-1
8.2 SLICE OPERATION OF 3D DATA 8-2
8.2.1 How to Use 3 D Slicer 8-2
8.2.2 How to Use 3D Slice Plotter 8-4

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8.1 DISPLAY OF 3D DATA

To display of the 3-dimensional data, the **3D Viewer** window or the **Data Slate** window is used.

8.1.1 3D Viewer Window

In the **3D Viewer** window, the slice or projection data for each axis of 3D data is arranged the same as in the **2D Viewer** window. You can specify an expansion area and a slice position in every display area.

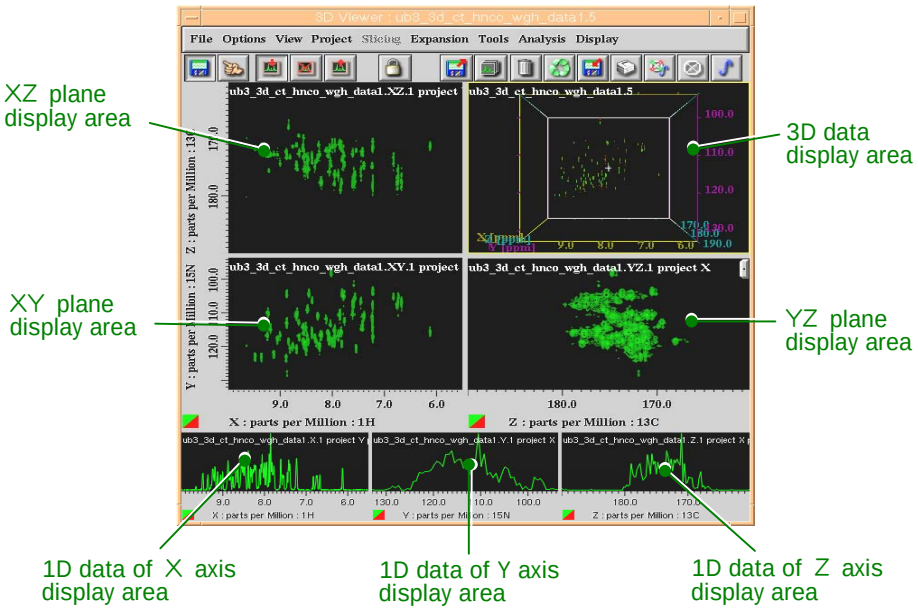
XZ plane display area
3D data display area
XY plane display area
YZ plane display area
1D data of X axis display area
1D data of Y axis display area
1D data of Z axis display area

Fig. 8.1 3D Viewer window

8.1.2 Data Slate Window

If you display 3D data in the **Data Slate** window, a 3D cube is displayed.

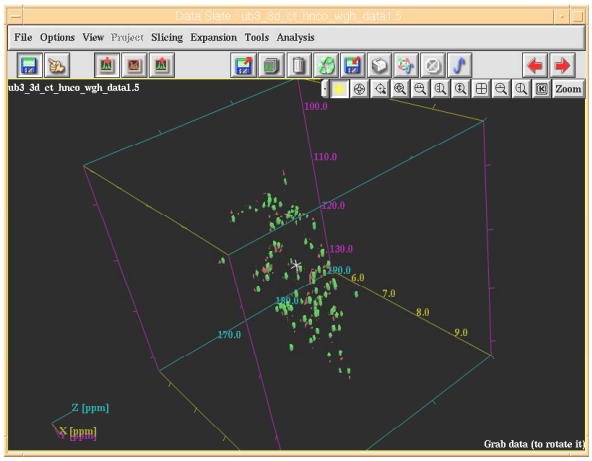

Fig. 8.2 3D Slate window

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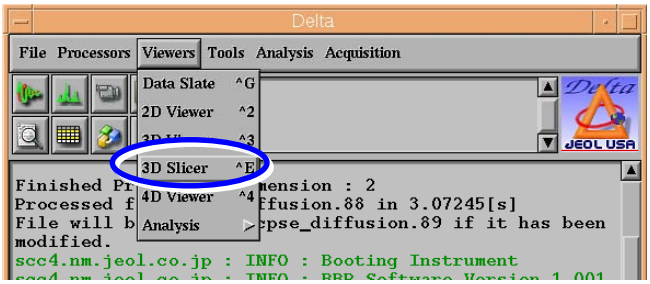
8.2 SLICE OPERATION OF 3D DATA

It is necessary to display or print many slice data for analyzing the 3D data. The **3D Viewer** window and the **Data Slate** window are not fit for such work. In these processes, you can use the **3D Slicer** window or the **3D Slice Plotter** window.

8.2.1 How to Use 3D Slicer

3D Slicer has two functions. One method extracts the two-dimensional spectrum that is slice perpendicular to any specific position in the 1D data projected on any axis; the other method extracts the one-dimensional spectrum perpendicular to the specified position in the 2D data projected on any plane. The projection axis and plane can be selected arbitrarily.
For example, in order to display the XZ slice plane at the specified point on the Y-axis, operate as follows.

1. Select **Viewers**–**3D Slicer** from the menu bar of the **Delta Console** window.



The **3D Slicer** window opens.

2. Read 3-dimensional data into the **3D Slicer** window.

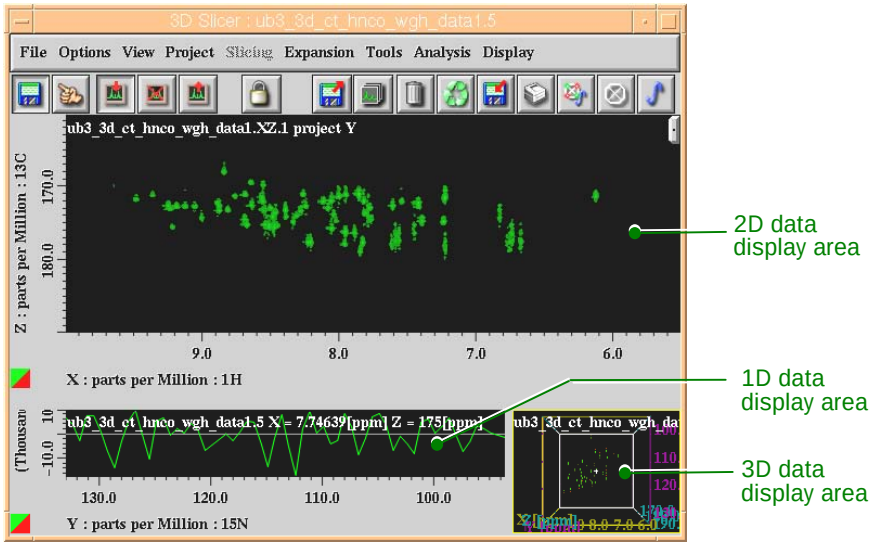
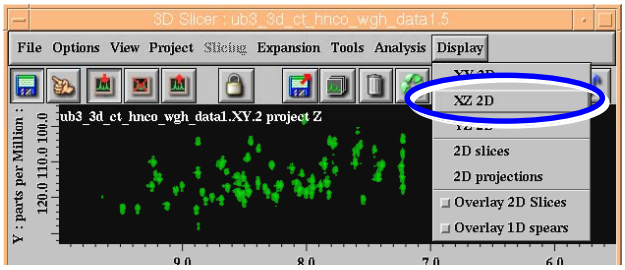

File Options View Project Slicing Expansion Tools Analysis Display
ub3_3d_ct_hnco_wgh_data1.XZ.1 project Y
Z : parts per Million : 13C
X : parts per Million : 1H
Y : parts per Million : 15N
2D data display area
1D data display area
3D data display area

Fig. 8.3 3D Slicer window

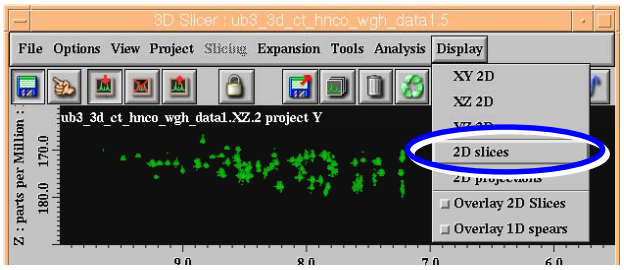
C I

3. Select **Display-XZ 2D** from the menu bar of the **3D Slicer** window.



The projection data on the XZ plane is displayed in the 2D data display area.

4. Select **Display–2D Slices** from the menu bar of the **3D Slicer** window.



The slice data of XZ plane is displayed in the 2D data display area. At this time, the data of the 1D data display area changes to the projection data on Y axis.

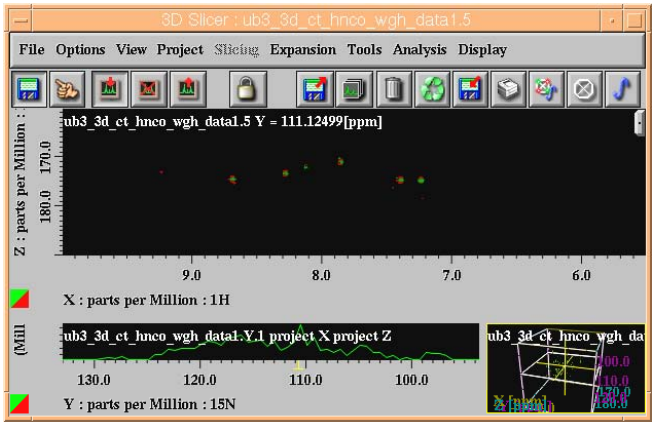
5. Determine a slice position as follows.

a. Select **Pick** mode using the cursor tool of the 1D data display area.

b. Click on the **Pick position** button in the **Pick** mode.

c. Click at a position to slice in the 1D data display area.

The pick position marker is displayed at the position where you clicked, and a slice plane is displayed in the 2D data display area.



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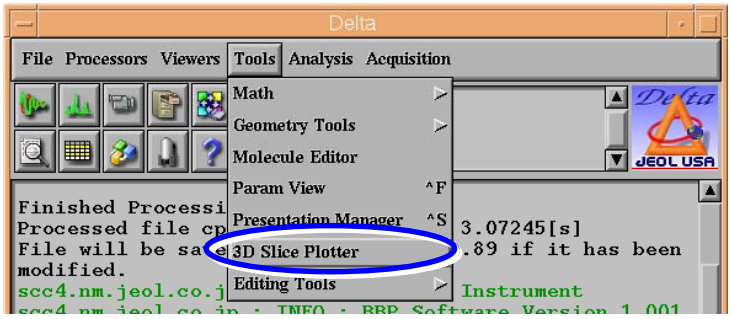
8.2.2 How to Use 3D Slice Plotter

3D Slice Plotter specifies a slice position in the projection data, and prints out the slice data. You can also display the slice data on a new **Data Slate** window without printing**.** For example, in order to specify and print XZ plane data at some points of the Y-axis, operate as follows.

1. Select **Tools–3D Slice Plotter** from the menu bar of the **Delta Console** window.



The **3D Slice Plotter** window opens.

2. Read 3D data into the **3D Slice Plotter** window.
1D projection data is displayed in the data display area.

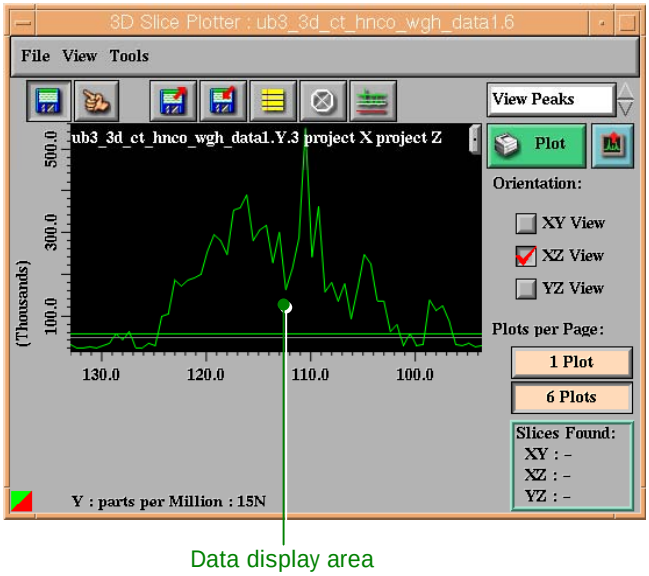


Fig. 8.4 3D Slice Plotter window

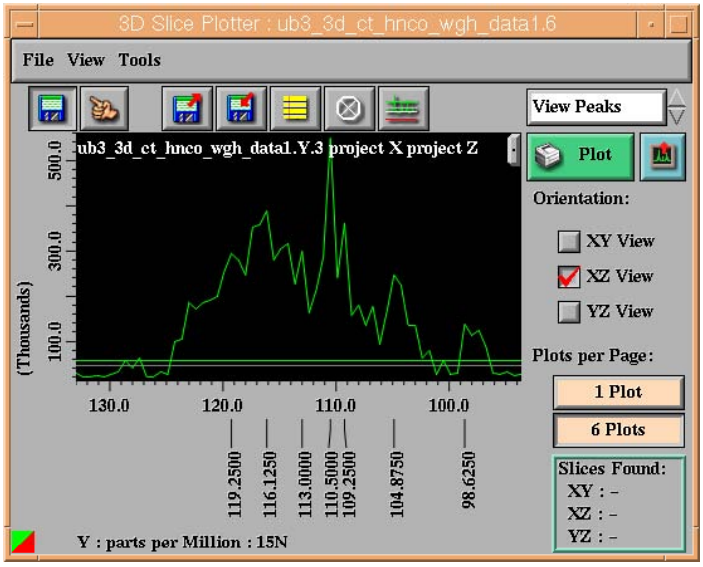
3. Put a check mark in **XZ View** in **Orientation** of the **3D Slice Plotter** window.
Y-axis projection data appears in the data display area.

4. Determine the slice position as follows.

a. Select **Peak** mode using the cursor tool of the data display area.

b. Click on the **Force create peak** button in the Peak mode.

c. Click a position to slice in the data display area.
A peak position marker appears at a slice position.



5. Specify the number of slice planes to print on one sheet of paper in **Plots per Page** of the **3D Slice Plotter** window.

1 Plot : One slice plane is printed on one sheet.

6 Plots : 6 slice planes are printed on one sheet.

6. Click on the Plot **Plot Slices Checked in Orientation below** button in the **3D Slice Plotter** window.

The slice plane of the specified slice position is printed.

Click on the **Show Slices in a Data Slate** button. A slice plane is displayed in a new **Data Slate** window. However, specification of **Plots per Page** is not possible in this case.

HOW TO USE PROCESSING FUNCTIONS

The Delta program provides various functions for data processing. Here, various processing functions are explained the order in which they appear in the pull-down menu of 1D and nD processing window.

9.1 PRE TRANSFORM 9-1
9.2 WINDOW 9-3
9.3 TRANSFORM 9-4
9.4 POST TRANSFORM 9-5
9.5 DISPLAY 9-7

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9.1 PRE TRANSFORM

Item	Explanation
Adaptive High Pass	Performs adaptable high pass filter. **Order**: Order of filter **Width** : Spectrum width **Center** : Center frequency of a spectrum
Auto N filter	Applies notch filter automatically based on offset value.
Auto Process	Performs basic processing such as peak picking and integration automatically.
Blip	Performs backward linear prediction based on LPSVD (Linear Prediction Singular Value Decomposition). **Order**: The order of the operation **Sample**: Number of points to sample from the file. **Reconstruct**: Number of points in the file to reconstruct.
DC Balance	Eliminates the signal at 0 Hz, which arises from the DC offset.
Decimate	Reduces the number of data points in order to perform digital filtering. **Factor**: Ratio of number of data points to keep to number of data points in the original data set. **Center**: Shift the center frequency by specified numerical value.
Diagonal Filter	Eliminates the signals near diagonal peaks in 2 D data. **K**: Specify K factor in the range from 1 to 128.
Elliptic	Performs Ellipse II R filter in the range specified by **Start** and **Stop**. It is applied to FID.
Filter Largest	Eliminates the largest peak in the specified range by filtering. **Center**: Specified value for center. **Width**: Specified value for width. **K**: K factor
Flip	Performs forward linear prediction. **Order**: The order of operation
FTS	Creates a data file consisting of original data from which noise is artificially eliminate. **No.Peaks**: Specifies a number of peaks to extract. **Threshold**: Specifies threshold. **Extend**: Expansion ratio.
FTS Automatic	Performs FTS automatically.
Gauss Echo Shift	Performs Gaussian window and its shift value. **Width** : Spectrum width

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Item	Explanation
High Pass	Performs high-pass digital filter. **K**: K factor
Inverse Chebyshev	Performs **Inverse Chebyshev IIR** digital filter in the range specified by **Start** and **Stop**.
Linear Prediction	Performs linear prediction. **Order**: The order of the operation. **Sample**: Number of points to sample from the file. **Reconstruct**: Number of points in the file to reconstruct.
Notch Filter	Performs notch filtering at the point specified by **Shift value.** **K**: K factor
PN to SHR	Transforms P/N type 2D data to States-Haberkorn-Ruben type data.
SHR to PN	Transforms States-Haberkorn-Ruben type data to P/N type data.
Shift	Shifts data by the number of position specified values by **Shift.**
Zero fill	Performs zero filling times N for the specified values by **Times**.

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9.2 WINDOW

Item	Explanation
Blackman	Applies Blackman window function.
Blackman-Harris	Applies Blackman-Harris window function.
Double Exponential	Applies Double Exponential window function. You can specify Lorentzian or Gaussian parameters.
GAUSS	Applies gaussian window function which is specified **Width** and **Shift**.
Hamming	Applies Hamming window function.
Kaiser	Applies Kaiser window function which is specified by π **Units**.
Single Exponential	Applies Single Exponential window function with specified **Width.** You can also specify **Shift** value.
Single Exponential Automatic	Performs Single Exponential window function, setting the parameters automatically by specifying **decay rate** with **Factor**.
Sinebell Automatic	Applies Sinebell window function by setting the parameters automatically.
Sinebell	Applies Sinebell window function with specified **Shift** and **Size.**
Sinebell (order 2)	Applies Sinebell (order 2) window function with specified **Shift** and **Size.**
Sinebell (order 4)	Applies Sinebell (order 4) window function with specified **Shift** and **Size.**
Sinebell Shift	Applies N shifted Sinebell window function with specified π/n value.
Traf	Applies Traf window function with specified **width** and **Shift.**
Traf Modified	Applies Traf window function with specified **width**, **Shift** and **Pre-Slope.**
Trapezoid	Applies trapezoidal window function with specified P1,P2 and P3.
Trapezoid 3	Applies trapezoidal window function with specified P2,P3 and P4.

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9.3 TRANSFORM

Item	Explanation
DOSY	Processing algorism of DOSY measurement data. **CONTIN**: Continuous type inverse Laplace transformation. This is suitable for the data of a system with a continuous molecular weight. **L-Marquardt**: Nonlinear curve fitting. This is suitable for the data with few overlaps of a peak. **MCR**: Multivariate Curve Resolve method This feature is that setting parameters for a calculation beforehand is few. **MCR-CONTIN**: Combination of the MCR and CONTIN **MCR-LM**: Combination of the MCR and L-Marquardt method. **MCR-SPLMOD**: Combination of the MCR and SPLMOD method. **SPLMOD**: Separation type inverse Laplace transformation. This is suitable for the data with which the different component peaks overlapped.
FFT	Fourier transforms. **Scale**: Sets multiplier for the first data point of FID. **Clip**: For the measured data after digital filtering, it is usually set to TRUE. In case of TRUE, the number of data points is reduced after Fourier transformation.
Hilbert	Hilbert transforms: Creates an imaginary data set from a real frequency-domain data set.
IFFT	Inverse Fourier transforms.
Maximum Entropy	Creates Frequency domain data from time domain data using Maximum Entropy method. Specify Times, Normal values and Noise values.
NMR Pipe	Transforms NMR Pipe format data and prints out to specified file.
SHEAR	Performs SHEARING processing for the 2D data measured by MQ-MAS method.
Transpose	Transposes matrix data. This cannot be applied for 1D data.

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9.4 POST TRANSFORM

Item	Explanation	
Abs	Transforms data to absolute-value data.	
Baseline Correction	**Base Correct**:	Corrects base-line rolling automatically.
	Division:	Select from None, Water or Cosy as the processing type.
	n Width:	Number of data points to process.
	Base Correct Interactive: Correct Base-line manually. Refer to the section 2.2.6 of User's manual " Processing"	
Clip	Reduces sampling points. Usually, it is applied to digitally filtered data.	
DC Correct	Adjusts DC offset level.	
Invoke	Starts a Percival program.	
Math	**Log**:	Performs base 10 logarithm (common logarithm)
	Real:	Only the real part of the data
	Real Format:	Creates a file of only the real part of the data.
	Reorder:	Changes the dimension of the file.
	Reverse:	Transposes data points symmetrically to center point.
Phase	**Apply Phase**:	Applies P0, P1 and PP, which are set to numerical values, to actual data file.
	Automatic Phase:	Corrects phase by P0 and P1 automatically. When Hold P1 is set to TRUE, the phase is corrected by only P0.
	Machine Phase:	Considering pulse duration, filter type, filter band width, dead time and delay time, corrects phase automatically.
	Digital Filter Phase:	Correct for phase distortion caused by digital filter to the original phase.
	Phase Exclude:	Eliminates the information for data specified by Center and Width, and corrects phase automatically considering pulse duration, filter type, filter-band width, dead time and delay tim.
Reference Deconvolution	Performs Deconvolution with Lorentzian for the peak which is specified Center, Width and Line_Width.	
Ridge	Detects a ridge and eliminates it in the range which is specified by StartCoord and StopCoord.	
Scale	Adjusts the scale to the specified value.	
Smooth	Performs smoothing processing.	
Sub Set	Selects a part of the data, and outputs it. Select dimension with **Dim;**	

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Item	Explanation
	specify the range by **Star**t and **End**.
Symmetrize	Performs symmetrization. Select Cosy, J-Resolve, Inadequate and Filter for processing type. Moreover, specify Threshold.
Tilt	Performs Tilt processing with specified Angle value.
Zero Region	Replaces the region specified by **Start** and **Stop** with ZERO or NOIZE.

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9.5 DISPLAY

Item	Explanation	
Bell	Rings a bell.	
Copy	Copies the file whose name is specified.	
Copy Data	Copies the data to specified directory.	
Display Signal / Noise	Displays SN value calculated by specified method for specified range in the **Delta Console** window.	
Display window	Displays a processed data in the **Data Slate** window.	
Export File	Transforms the data to the specified file format, and outputs it in the foreign_data directory.	
Hertz	Sets unit to Hertz.	
Integrals	**Apply Integral**:	Performs integration according to the integration range specified by Template File which is created by Transfer Integral Tool.
	Auto Integrate:	Automatically searches for the peaks specified by IntegWidth, and integrate them.
	Integrate Region:	Performs integration in the range which is specified by **Start** and **Stop**.
	Normalize Tallest Integral :	Sets **Normal** value to integration value of maximum peak, and performs the same processing as **Auto Integrate**.
	Normalize Smallest Integral :	Sets **Normal** value to integration value of minimum peak, and performs the same processing as **Auto Integrate**.
Peaks	**Auto Peak Pick**:	Performs automatic peak picking with the values specified by J-coupling.
	Deconvolve:	Performs deconvolution.
	Peak Chop:	Chops the n tallest peaks to the height of the (n+1)st tallest peak, if the (n+1)st tallest peak is less than maximum percent as tall as the tallest peak.
	Peak Limit:	Restricts the number of peak picks to the number specified by **Limit**.
	Solvent peak limit:	Omits solvent peaks or reference peak.
Peak Pick / Integrate	Performs peak picking automatically with the value specified by J-coupling, detects the peaks having peak width specified by **IntegWidth**, and integrates them.	
Play	This is not used.	
Plot	**Plot**:	Prints.
	Presentation Plot:	Prints with the format specified by Presentation Manager.
	Plot Expand Integrals:	This is not used.

Item	Explanation	
	Print Integral List:	Prints integrations list.
	Print Peak List:	Prints peak lists.
PPM	Set unit to ppm.	
Reference	**Automatic Reference**:	Sets reference automatically.
	Copy Reference:	Specifies source list, and copies the reference information.
	Maximum Reference:	Detects the maximum peak in the range specified by **Ref** and **Width**, and sets the reference specified by **Ref** to the detected peak.
	Reference:	Sets the value specified by **Reference** to the position specified by **Position**.
	Unreference:	When a reference has already been set, returns to the original state.
	Linear Reference:	Sets the reference specified by Center position to Beta. Moreover, expands scale by the value specified by Alpha.
Save	Saves the processed data with the name specified by Filename.	
Stop	Stops data processing.	
Threshold	Expands threshold level with the value specified by Multi.	
TSC Database	Creates TSC data base file.	

10

DISPLAY FUNCTIONS OF PROCESSING DATA

If you click the right button on a data processing screen such as 1D Processor, Data Slate and 2D Viewer, a pop up menu appears. Here, the contents of the pop up menu are explained. The displayed items change according to the display window, existence of the cursor tool display, and set-up **Mode Class**.

10.1 POP UP MENU OF 1D DATA SCREEN 10-1
10.1.1 When Cursor Tool is not being Displayed 10-1
10.1.2 When Cursor Tool is being Displayed 10-5
10.1.3 Setting Each Item 10-7
10.2 POP-UP MENU IN TWO-DIMENSIONAL DATA SCREEN 10-19
10.2.1 When Cursor Tool is not being Displayed 10-19
10.2.2 When Cursor Tool is being Displayed 10-23
10.2.3 Setting Each Item 10-26

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10.1 POP UP MENU OF 1D DATA SCREEN

The pop-up menu displayed on the 1D data screen of 1D Processor, DataSlate and 2D Viewer is explained below.

10.1.1 When Cursor Tool is not being Displayed

When the cursor tool is not being displayed (it is minimized), if you click the right button of the mouse on the geometry of **1D Processor** or **Data Slate** window, a pop-up menu as shown in Fig. 10.1 appears.

The cursor tool can be displayed by clicking its tab button or right clicking-**Option–Display–Show Cursor Tool**.

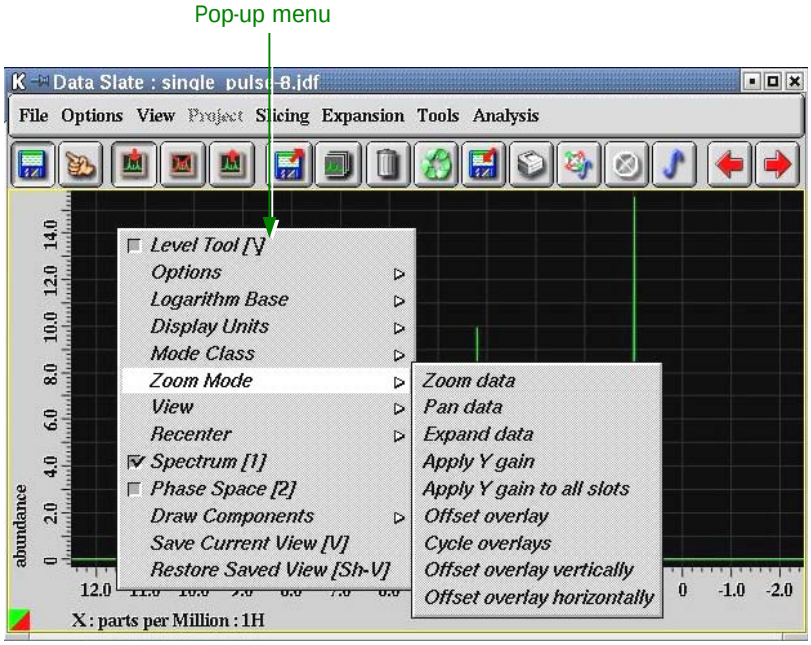

Fig. 10.1 Pop-up menu when Mode Class set to Zoom

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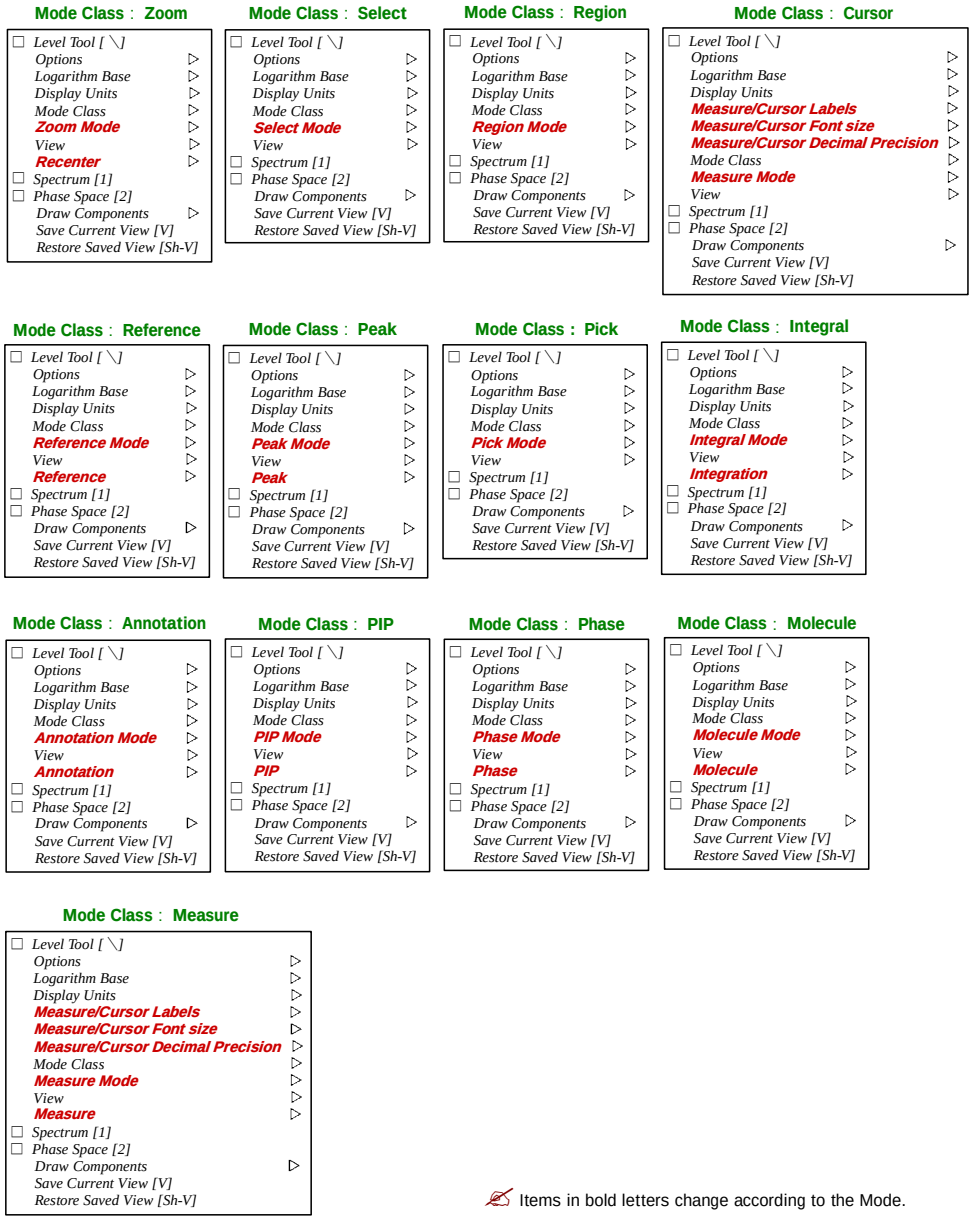
Pop-up menu for every Mode Class setting

The pop-up menu changes with the setting of **Mode Class** (Fig. 10.2).



Items in bold letters change according to the Mode.

Fig. 10.2 Pop-up menu when the cursor tool is not displayed

Menu items

Item	Explanation	Display of item
Level Tool [\ ]	Displays the level tool.	All mode
Options	Sets the display item.	
Logarithm Base	Changes the unit for logarithm display.	
Display Units	Changes a unit of the X axis.	
Measure/Cursor Labels	Changes the setting item for **Cursor** and **Measure.**	**Measure/ Cursor** mode
Measure/Cursor Font Size	Changes the font size for displaying **Cursor** and **Measure.**	
Measure/Cursor Decimal Precision	Changes the decimal points position for displaying Cursor and Measure.	
Color of Selected Object	Changes the color of the selected text.	**Annotation** mode (when text appears)
Font of Selected Text	Changes the font of the selected text.	
Size of Selected Text	Changes the font size of the selected text.	
Attribute of Selected Text	Changes the character style of the selected text.	
Outline of Selected Text	Changes the outline of the selected text.	
Rotation of Selected Text	Changes the direction of the selected text.	
Mode Class	Changes the cursor.	All mode
Zoom Mode	Changes various setting items in **Zoom** mode.	**Zoom** mode
Select Mode	Changes various setting items in **Select** mode.	**Select** mode
Region Mode	Changes various setting items in **Region** mode.	**Region** mode
Cursor Mode	Changes various setting items in **Cursor** mode.	**Cursor** mode
Reference Mode	Changes various setting items in **Reference** mode.	**Reference** mode
Peak Mode	Changes various settings in **Peak** mode.	**Peak** mode.
Pick Mode	Changes various settings in **Pick** mode.	**Pick** mode
Integral Mode	Changes various settings in **Integral** mode.	**Integral** mode
Annotation Mode	Changes various settings in **Annotation** mode.	**Annotation** mode
PIP Mode	Changes various settings in **PIP** mode.	**PIP** mode
Phase Mode	Changes various settings in **Phase** mode.	**Phase** mode
Molecule Mode	Changes various settings in **Molecule** mode.	**Molecule** mode
Measure Mode	Changes various settings in **Measure** mode.	**Measure** mode
View	Expands, reduces and resets for display.	All mode
Reference	Changes setting values for **Reference** mode**.**	**Reference** mode
Peak	Changes setting values for **Peak** mode.	**Peak** mode
Integration	Changes setting values for **Integration** mode.	**Integration** mode
Annotation	Changes the note set in the **Annotation** mode.	**Annotation** mode

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Item	Explanation	Display of item
PIP	Changes setting values for **PIP** mode.	**PIP** mode
Recenter	Changes setting values for **Zoom** mode.	**Zoom** mode
Phase	Changes setting values for **Phase** mode.	**Phase** mode
Molecule	Changes setting values for **Molecule** mode.	**Molecule** mode
Measure	Changes setting values for **Measure** mode.	**Measure** mode
Spectrum [1]	Displays an ordinary spectrum	All mode
Phase Space [2]	The figure which shows phase sensitive data is displayed from the x axis direction.	
Draw Components	Selects either data display real or imaginary.	
Save Current View [V]	Saves the area currently displayed.	
Restore Saved View [Sh-V]	Returns to the original state.	

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10.1.2 When Cursor Tool is being Displayed

When the cursor tool is being displayed, if you click the right button of the mouse on the geometry of **1 D Processor** or **Data Slate** window, a pop-up menu as shown in Fig. 10.3 appears.

✍ The cursor tool can be displayed by clicking its tab button or right clicking-**Option–Display–Show Cursor Tool**.

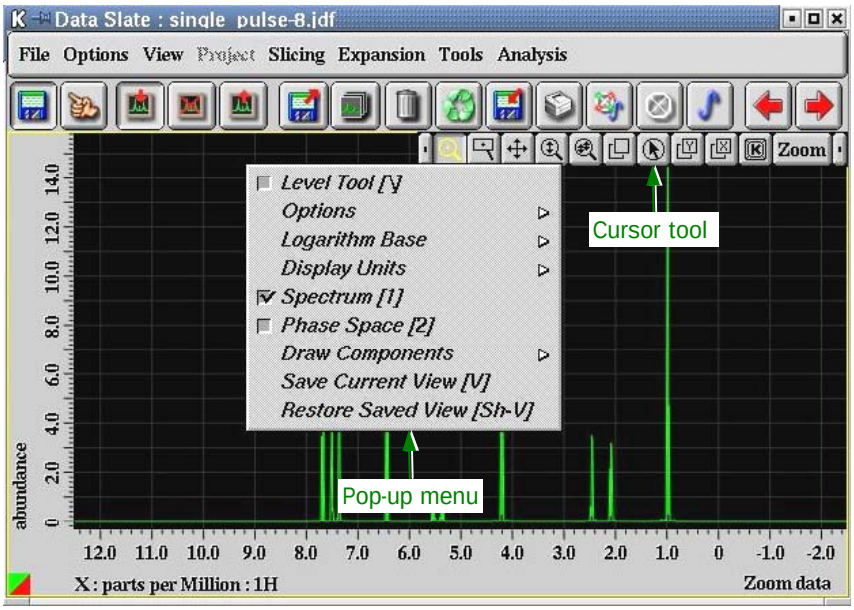

Fig. 10.3 The pop up menu for cursor tools other than Cursor and Measure.

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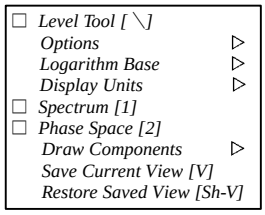
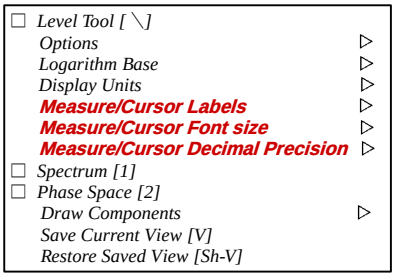
Pop-up menus for every display mode

When the cursor tool is set to **Measure** or **Cursor**, the pop-up menus differ from those in other Modes.

Modes other than **Cursor** and **Measure** mode



In Cursor and **Measure** mode



Items in bold letters differ according to mode

Fig. 10.4 Pop up menu when the cursor tool is being displayed

Menu items

Item	Explanation	Display of item
Level Tool [\ ]	Displays the level tool.	All modes
Options	Sets the display item	
Logarithm Base	Changes a unit for logarithm display.	
Display Units	Changes a unit of the X axis.	
Measure/Cursor Labels	Changes setting item for **Cursor** and **Measure.**	**Measure/ Cursor** mode
Measure/Cursor Font Size	Changes the font size for displaying **Cursor** and **Measure.**	
Measure/Cursor Decimal Precision	Changes the position of decimal points for displaying **Cursor** and **Measure**.	
Spectrum [1]	Displays an ordinary spectrum.	All modes
Phase Space [2]	The figure shows phase sensitive data displayed from the x axis direction.	
Draw Components	Selects either data display of real or imaginary.	
Save Current View [V]	Saves currently displayed range.	
Restore Saved View [Sh-V]	Returns to original state.	

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10.1.3 Setting Each Item

The items on the display differ according to the display window, whether the cursor tool is displayed or hidden, and the present **Mode Class**.

Options

Item	Explanation	
Annotations [Alt-A]	Displays the notes which are set in the **Text** mode.	
Cursors [Alt-C]	Displays the cursor which is set in the **Cursor** mode.	
Measures [Sh-Alt-H]	Displays the measuring range which is set in the **Measure** mode.	
PiP Windows [Alt-W]	Displays the area of the **PIP** box which is set in the **PIP** mode on the spectrum.	
Regions [Alt-R]	Displays the area which is set in the **Region** mode.	
Integral	**Integrals [Alt-I]:**	Displays the integration curves which are set in the **Integral** mode.
	Integral Value [Alt-Q]:	Displays the integration curves.
	Peak Integration [Alt-E]:	Integrates the peaks which are picked up.
Peak	**Center of Mass [Sh-Alt-W]:**	Calculates the center of the peak from the integration values and peak positions of two peaks, and display it.
	Deconvolve [Alt-K]:	Displays the result of deconvolution.
	Deconvolve Sum [Alt-H]:	Displays the spectra obtained by deconvolution.
	Deconvolv Unselected [Sh-Alt-K]:	Displays all results obtained by deconvolution.
	Draw Peaks [Sh-Alt-U]:	Draws a triangle on the peaks selected in the peak picking.
	Draw Unselected peaks [Sh-Alt-V]:	Draws a triangle on the peaks unselected in the peak picking.
	Peak Above [Alt-U]:	Displays peak-position makers and chemical shift values above the peaks.
	Peak Pick [Alt-P]:	Displays the peak information when in any mode other than Peak mode.
	Sequence [Alt-J]:	Displays the peak information which is set using spreadsheet.
Molecule	**Atom Numbers [Sh-Alt-A]**	Numbers the skeleton of molecular structural formula which is displayed on the geometry.
	Atom Select Numbers [Sh-Alt-S]:	Numbers the selected skeleton.
	Atom Sequence [Sh-Alt-Q]:	Displays the correlation between the selected skeleton and peaks.

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Item	Explanation	
	Molecules [Sh-Alt-M]:	Displays the structure set in the molecular mode when displaying in any mode other than Molecular mode.
	Molecule Border [Sh-Alt-D]:	Displays a frame on the molecule.
	Molecule Titles [Sh-Alt-T]:	Displays the title of molecule.
Data	**Data [Alt-D]:**	Displays data.
	Data Points[Alt-N]:	Displays the marker on each data points.
	Center Contour Levels Around Baseplane:	In 2 D data display, redisplays the data based on the statistics which are set initially.
	Statistics [Alt-T]:	Displays base level, noise level and threshold level of peak.
	Trace Model [Sh-Alt-L]:	In linearized display of a selected peak, points near the peak top are connected by a smooth curve.
	Trace Profile [Sh-Alt-F]:	In linearized display of a peak, points near the peak top are connected by lines.
	Extra Data Color solid:	An appropriate color is used for the projection of 2D/3D space.
	Phase Value Maintained Step to Step:	Keeps the phase values.
Display	**Grid[Alt-G]:**	Displays grid lines.
	PIP Border[Alt-S]:	Display the frame of the PIP box.
	Plot Border[Sh-Alt-B]:	Display the frame of the Plot box.
	Plot Transparent[Alt-I]:	The part of the main spectrum which overlaps PIP box is also printed.
	Plot Zero Line:	Displays a line for the zero level.
	Overlay Tabs[Sh-Alt-O]:	In overwrite, displays tab in which selects spectrum.
	Scan To Threshold [Sh-Alt-R]:	When you want to search a slice data set automatically using threshold level, turn this on.
	Show Cursor Tool [Tab]:	Displays cursor tool.
File Information	**All overlays[Alt-O]:**	In overwriting, displays file names of all spectra.
	Comment [Sh-Alt-C]	Displays comment.
	File Name [Alt-F]	Displays file name.
	Shadow Dimensions [Alt-B]:	Displays the position of a slice data set by point, percent or second.
Ruler	**X Ruler [Alt-X]:**	Displays X axis.
	Y Ruler [Alt-Y]:	Displays Y axis.

Item	Explanation	
	Logarithmic X Ruler [Sh-Alt-X]:	Displays X axis with logarithmic scaling.
	Show Number of Points [Sh-Alt-E]:	Displays point numbers on X axis.
	Show Ruler Type [Sh-Alt-E]:	Display ruler type on X axis.
	Display Clock Time:	Displays with human time.

Logarithm Base

Item	Explanation
2	Displays as base two logarithms.
e	Displays as natural logarithms.
10	Displays as common logarithms.

Display Units

Item	Explanation
Hertz	Displays X axis in Hertz.
ppm	Displays X axis in ppm.
Percent	Displays X axis in percent.
Points	Displays X axis in points.
Peak Units	**Hertz:** Displays the chemical shift of picked peak in Hertz. **ppm:** Displays the chemical shift of picked peak in ppm. **Percent**: Displays the chemical shift of picked peak in percent. **Points**: Displays the chemical shift of picked peak in points. **Ruler Units**: Displays the chemical shift of picked peak in the same unit as that of X axis ruler.
Measure/Cursor Unit	**Hertz**: Displays the unit of measuring range as Hertz. **ppm**: Displays the unit of measuring range as points. **Percent**: Displays the unit of measuring range as percent. **Points**: Displays the unit of measuring range as points. **Ruler Units**: Displays the unit of the peak pick in the same unit as that of X axis ruler.
Reset	Returns to the initial settings.
Cycle	Returns to the settings of one step before.

Measure/Cursor Labels

Item	Explanation
Show Measure X	Shows measuring range.

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Item	Explanation
Show Measure Amplitude	Shows measuring range.
Show Measure All	Shows information about unselected measuring range.
Show Measure None	Does not show information about an unselected measuring range.

Measure/Cursor Font Size

Item	Explanation
6～38	Changes the font size in a range from 6 to 38.
Default	Sets the font size to the default value.

Measure/Cursor Decimal Precision

Item	Explanation
1～12	Changes decimal places in a range 1 to 12 digits.
Default	Sets decimal places to the default value.

Draw Components

Item	Explanation
Draw Real [Sh-1]	Displays real data.
Draw Imag [Sh-2]	Displays imaginary data.

Mode Class

While the cursor tool is on the display, these modes can be changed on the cursor tool.

Item	Explanation
Zoom [F1]	Changes to **Zoom** mode.
Select [F2]	Changes to **Select** mode.
Region [F3]	Changes to **Region** mode.
Cursor [F4]	Changes to **Cursor** mode.
Reference [F5]	Changes to **Reference** mode.
Peak [F6]	Changes to **Peak** mode.
Pick [F7]	Changes to **Pick** mode.
Integral [F8]	Changes to **Integral** mode.
Annotation [F9]	Changes to **Annotation** mode.
PiP [F10]	Changes to **PIP** mode.
Phase [F11]	Changes to **Phase** mode.

Item	Explanation
Molecule [F12]	Changes to **Molecule** mode.
Measure [Print Scrn]	Changes to **Measure** mode.

View

When the cursor tool is on the display, these items are in the key command.

Item	Explanation
Reset View [Home]	In expand display, reset display area.
Reset All Dims Sh-Ctl-Home]	When displaying a datadex, irrespective of selection geometry, reset the display range in both X and Y axes.
Unzoom [Bksp]	Undoes last zoom.
Scale Y [End]	Adjusts length of Y axis of display range automatically.
Unscale X [Sh-End]	Resets X axis of display range.
Cycle Slot + [PgUp]	When overwriting, selects spectra in the overwritten order.
Cycle Slot – [PgDn]	When overwriting, selects spectra in the overwritten inverse order.
Pan –Y [Dwn]	In expand display, moves the spectrum downward.
[Pan +Y [Up]	In expanded display, moves the spectrum upward.
Pan –X [Lft]]	In expanded display, moves the spectrum leftward.
Pan +X [Rg+]	In expanded display, moves the spectrum right word.
Expand –Y [Ctl-Dn]	Reduces the display range along the Y axis.
Expand+Y [Ctl-Up]	Expands the display range along the Y axis.
Expand –X [Ctl-Lft]	Reduces the display range along the X axis.
Expand +X [Ctl-Rgt]	Expands the display range along the X axis.

Zoom Mode

Item	Explanation
Zoom data	Expands the surrounded area.
Pan data	Moves the spectrum in the vertical direction by the Y ruler and in the horizontal direction by the X ruler.
Expand data	Expands or reduces the spectrum in the vertical direction by the Y ruler and in the horizontal direction by the X ruler.
Apply Y gain	Expands and reduces the spectrum in the vertical direction.
Apply Y gain to all slots	Expands and reduces all the spectra overlapped in the vertical direction.
Offset overlay	Changes the display position in the vertical and horizontal direction for the selected spectrum from the overlapped spectra.
Cycle overlay	Displays the overlapped spectra.
Offset overlay in Y	While the spectra are displayed overlapping, changes the display position in the vertical direction.

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Item	Explanation
Offset overlay in X	While the spectra are displayed overlapping, changes the display position in the horizontal direction.

Select Mode

Item	Explanation
Select geometry	Selects a geometry for operation.
Cycle overlays	When overwriting spectra in the one geometry, selects the desired spectra.
Apply box analysis	When carrying out a certain operation on a limited area in one geometry, specifies the operation. For example, specify the range of application of **Zero Region** function in the **2D Viewer** window.

Region Mode

Item	Explanation
Create region	Specifies a domain at **PIP** box creation. Perform **BOX** in the **Presentation Manager** window, and specify a domain in the **2D Phaser**.
Move/Resize region	Moves the PIP box, and changes its size. Moves the **BOX** and changes its size in **the Presentation Manager** window.
Delete region	Deletes **PIP** box. Delete BOX in the **Presentation Manager** window.

Cursor Mode

Item	Explanation
Create cursor	Creates new cross cursor.
Move cursor	Moves the position of cross cursor.
Select cursor	Selects cross cursor.
Delete cursor	Deletes cross cursor.

Reference Mode

Item	Explanation
Grab position for reference	Takes a frequency of specified a spectrum into the computer as a reference frequency.
Paste reference	Pastes a reference frequency on the specified position.
Paste reference to nearest peak	Pastes the reference to the nearest peak from the specified position.
Paste reference to all geometries	Pastes the reference on the all geometry of overlay display.
Cycle overlays	Clicks on the geometry of overlay display, selecting geometry move to the next.

Reference

While the cursor tool is on the display, these items are in the key command.

Item	Explanation
Round [R]	Display as integers.
Zero [Z]	If you select this command in **Paste reference** before pasting reference, the peak selected in **Paste reference** becomes zero.

Peak Mode

While the cursor tool is on the display, these items are in the key command.

Item	Explanation
Create peak	Sets up the peak top near the position selected as a new peak.
Force create peak	Adds specified position as a peak.
Delete peak	Eliminates a peak.
Adjust peak threshold	Determines the detection peak level using the statistics set during peak picking.
Adjust noise threshold	Determines the noise level using the statistics set during peak picking.
Adjust baseplane / thresholds	Determines the base level using the statistics set during peak picking.
Select peaks	Selects the peaks set already.
Select more peaks	Selects more peaks when peaks are already selected.
Unselect peaks	Cancels peak selection.

Peak

While the cursor tool is on the display, these items are in the key commands.

Item	Explanation
Select All [A]	Selects all peaks.
Unselect All [U]	Cancels the selection of peaks.
Complement [C]	Switches selected peaks to unselected peaks and unselected peaks to selected peaks.
Delete [Del]]	Eliminates the selected peaks.
Undelete [Ins]	Undoes delete.
Normalize [N]	Makes a reference of the integration value of a selected peak for the integration.
Group peaks [G]	Displays the center of selected signal group.
Meld peaks [M]	Displays the center of selected peak.
J Coupling [J]	Displays the coupling constant of selected peaks.
Sequence Search [S]	Searches the spreadsheet information in analysis of protein.
Fit Lorentzian [L]	Performs curve fitting using a Lorentzian.
Fit Gaussian [F]	Performs curve fitting using a Gaussian.

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Item	Explanation
Fit Mixed [X]	Performs curve fitting with a function that combine Lorentzian and Gaussian.
Center of Mass [W]	Displays the peak center using an integration value and peak position.
Recompute Statistics [R]	Recalculates statistics which are set automatically.

Pick Mode

Item	Explanation
Pick position	Reads peak position.
Copy position to buffer	Copies the read peak positions.
Copy position of nearest peak to buffer	Copies the position of the nearest peak from the specified position.
Set datadex slice point	Sets slice spot for the extraction slice data to datadex.
Spear datadexed file	Displays peak position on the datadex.
Copy relative to center of ruler	Reads the distance between the selected peak and center of the spectrum, and places it in the paste buffer in the **Delta Console** window.
Pick lower Contour Bound	Sets the lowest level of contour map using the projection or slice data.
Pick Upper Contour Bound	Sets the top level of contour map using the projection or slice data.
Pick Selected Contour Threshold	Sets the contour level which is selected using the **Level Tool** window in the projection or slice data.

Integral Mode

Item	Explanation
Create integral	Sets a new integration range.
Delete integral	Deletes an integration range.
Change slope of integral	Sets the slope in the integration range. Correct it by changing base point marker.
Adjust integral	Adjusts an integration range.
Split integral into two	Separates two parts at an arbitrary point which is selected on the integration curve.
Gain integrals in Y	Sets a length in the vertical direction in the integration range.
Change offset of integrals	Sets the position of integration curve in the spectrum.
Adjust peak threshold	Adjusts peak-detection level with the statistics set during peak picking.
Adjust noise threshold	Adjusts noise level with the statistics set during peak picking.
Adjust baseplain / threshold]	Adjusts base-line level with the statistics set during peak picking.
Select integrals	Selects the integration ranges which have been set.

Item	Explanation
Select more integrals	Selects more integration ranges after some integration ranges are already selected.
Unselect integrals	Cancels the selected integration ranges.

Integration

While the cursor tool in on the display, these items are in the key commands.

Item	Explanation
Select All [A]	Selects all integration values.
Unselect All [U]	Cancels the selection.
Complement [C]	Interchanges the selected and the unselected signals.
Delete [Del]	Deletes the selected integration value.
Undelete [Ins]	Undoes deletion of integration values.
Normalize [N]	Sets selected integration values to the values which are set in the **Set Integral Normalize**.
Gain Select [G]	Sets selected integration gain.
Recompute Statistics [R]	Recalculates statistics which are set automatically.

Annotation Mode

Item	Explanation
Create text annotation	Inputs text (comment) on any place in the data-processing display area.
Edit text annotation	Changes the text.
Create Rectangle	Creates a rectangle any where in the data processing display area.
Create Line	Creates a line any where in the data processing display area.
Create Arrow	Creates an arrow any where in the data processing display area.
Create Double Arrow	Creates a two side arrow any where in the data processing display area.
Move/Resize Annotation	Moves text and changes its size.
Delete annotation	Deletes text.
Select annotation	Selects text.
Add select annotation	Selects more text while some text is already selected.
Unselect annotation	Cancels the selection.

Annotation

While the cursor tool is on the display, these items are in the key commands.

Item	Explanation
Select All [A]	Selects all text.
Unselect All [U]	Cancels the selected text.

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Item	Explanation
Complement [C]	Select every thing except the currently selected text.
Delete [Del]	Deletes the selected text.
Cycle Font For Selected [Sh-Dwn]	Changes the font of the selected text in the order of the item in **Font of Selected Text**
Cycle Font For Selected [Sh-Up]	Changes the font of the selected text in the reverse order of the item in **Font of Selected Text**
Cycle Size For Selected [Ctl-Dwn]	Changes the font size of the selected text in the order of the item in **Size of Selected Text**
Cycle Size For Selected [Ctl-Up]	Changes the font size of the selected text in the reverse order of the item in **Size of Selected Text**
Cycle Style Attribute For Selected [Alt-Dwn]	Changes the font style of the selected text in the order of the item in **Style of Selected Text**
Cycle Style Attribute For Selected [Alt-Up]	Changes the font style of the selected text in the reverse order of the item in **Style of Selected Text**

PIP Mode

Item	Explanation
Create PIP by zoom region	Creates PIP box (partial spectrum) from a whole spectrum.
Move/Resize PIP zoom region	Moves the PIP box and changes its size.
Create PIP	Inserts a whole spectrum at any place in the display area of processing data. Area of the spectrum inserted can be changed by **Zoom** mode.
Move/Resize PIP	Moves the PIP box created in **Create PIP** and changes its size.
Delete PIP	Deletes the PIP boxes.

PIP

While the cursor tool is on the display, these items are in the key commands.

Item	Explanation
Prettify [P]	Arranges the PIP boxes.

Phase Mode

Item	Explanation
Adjust the Phase PP value	Adjusts the display phase parameter (PP).
Adjust the Phase P0 value	Corrects the zero order phase parameter (P0).
Adjust the Phase P1 value	Corrects the first order phase parameter (P1).
Pick position	Reads a peak position.

Phase

Item	Explanation
Reset Phase P0 and P1 [R]	Resets the zero-order phase (P0) and first-order phase (P1) parameter value.
Reset Phase P0 [O]	Resets the P0 parameter value.
Reset Phase P1 [I]	Resets the P1 parameter value.
Reset Phase PP [P]	Resets the position of display-phase parameter PP.
Autophase 1D[A]	Performs automatic phase correction.
Apply Phase [Enter]	Adds the display-phase correction parameter value to the process list.
Apply Phase to Entire File [Ctl-Enter]	Adds the display-phase correction parameter value to the process list for the whole file.

Recenter

While the cursor tool is on the display, these are in the key commands.

Item	Explanation
Recenter [R]	In the overlay data, return only the selected data to the original position.
Recenter Def [D]	In the overlay data, return the display position of each data set to the positions in the **File—Preference** of the **Delta Console** window.
Recenter All [A]	In the overlay data, return to the original position.

Molecule Mode

Item	Explanation
Create Molecule window	Specifies a range when creating a **Molecule** window.
Move/Resize Molecule window	Moves the **Molecule** window and changes its size.
Select Molecule window	Selects the **Molecule** window.
Delete Molecules window	Deletes the **Molecule** window.
Select Atom	Selects atoms in the **Molecule** window.
Select more peaks	Selects more peaks.
Unselect peaks	Cancels peak selection.

Molecules

While the cursor tool is on the display, these items are in the key commands.

Item	Explanation
Attach to X [X]	Relates a displayed structural formula and the peaks of the spectrum.
Unattach to X [Sh-X]	Cancels the relation between a displayed structural formula and the peaks.
Unselect Attached Atoms	Cancels the selection of unrelated points of the structural formula.

Item	Explanation
[T]	
Unselect All Peaks [U]	Cancels selected points on structural formula related with all peaks.
Save Molecule File [S]	Saves displayed structural formula.

Measure Mode

Item	Explanation
Create Measure	Sets the measuring range.
Create Measure in X	Specifies a measurement range in the X direction.
Create Measure in Y	Specifies a measurement range in the Y direction.
Resize Measure	Changes the measuring range.
Resize Measure in X	Changes the measurement range in the X direction.
Resize Measure in Y	Changes the measurement range in the Y direction.
Rotate Measure	Changes the direction of measuring range.
Select Measure Near Cursor	Selects the measuring range which is set.
Unselect Measure	Cancels the selected measuring range.
Delete Measure	Cancels the selected measuring range.

Measure

While the cursor tool is on the display, these items are in the key commands.

Item	Explanation
Unselect [U]	Cancel the selected measuring range.
Delete Selected [D]	Deletes the selected measuring range.
Delete All [R]	Deletes all measuring ranges.
Display All [D]	Displays the measuring range and all information.

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10.2 POP-UP MENU IN TWO-DIMENSIONAL DATA SCREEN

Here the pop-up menu displayed on the2D data screen of **Data Slate** and 2**D Viewer** is explained.

10.2.1 When Cursor Tool is not being Displayed

When the cursor tool was not being displayed, if you click right button of the mouse on the geometry of **Data Slate** or **2D Viewer** window, a pop-up menu as shown in Fig. 10.5 appears.

The cursor tool can be displayed by clicking on its tab button or by right clicking-**Option–Display–Show Cursor Tool**.

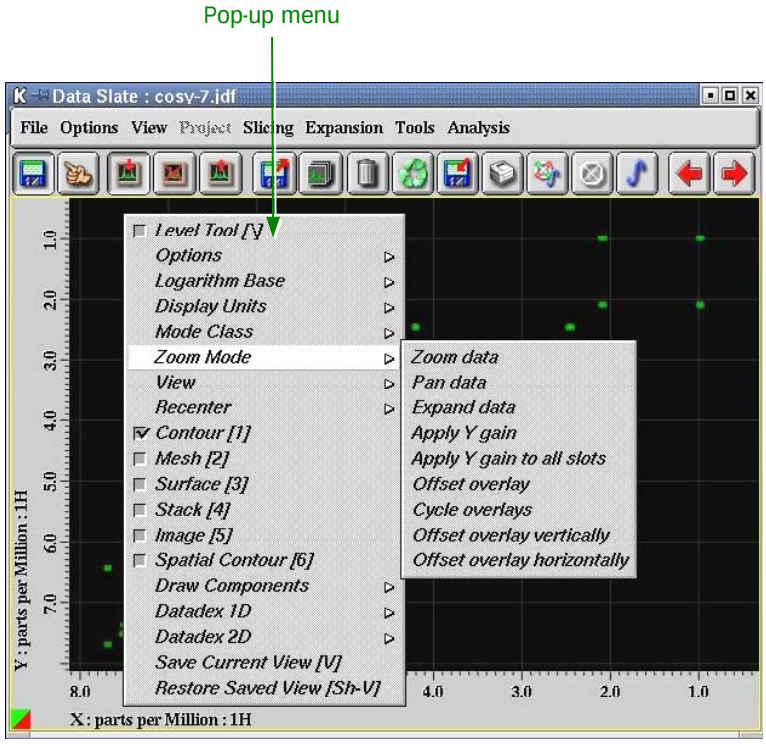

Fig. 10.5 Pop-up menu when Mode Class set to Zoom

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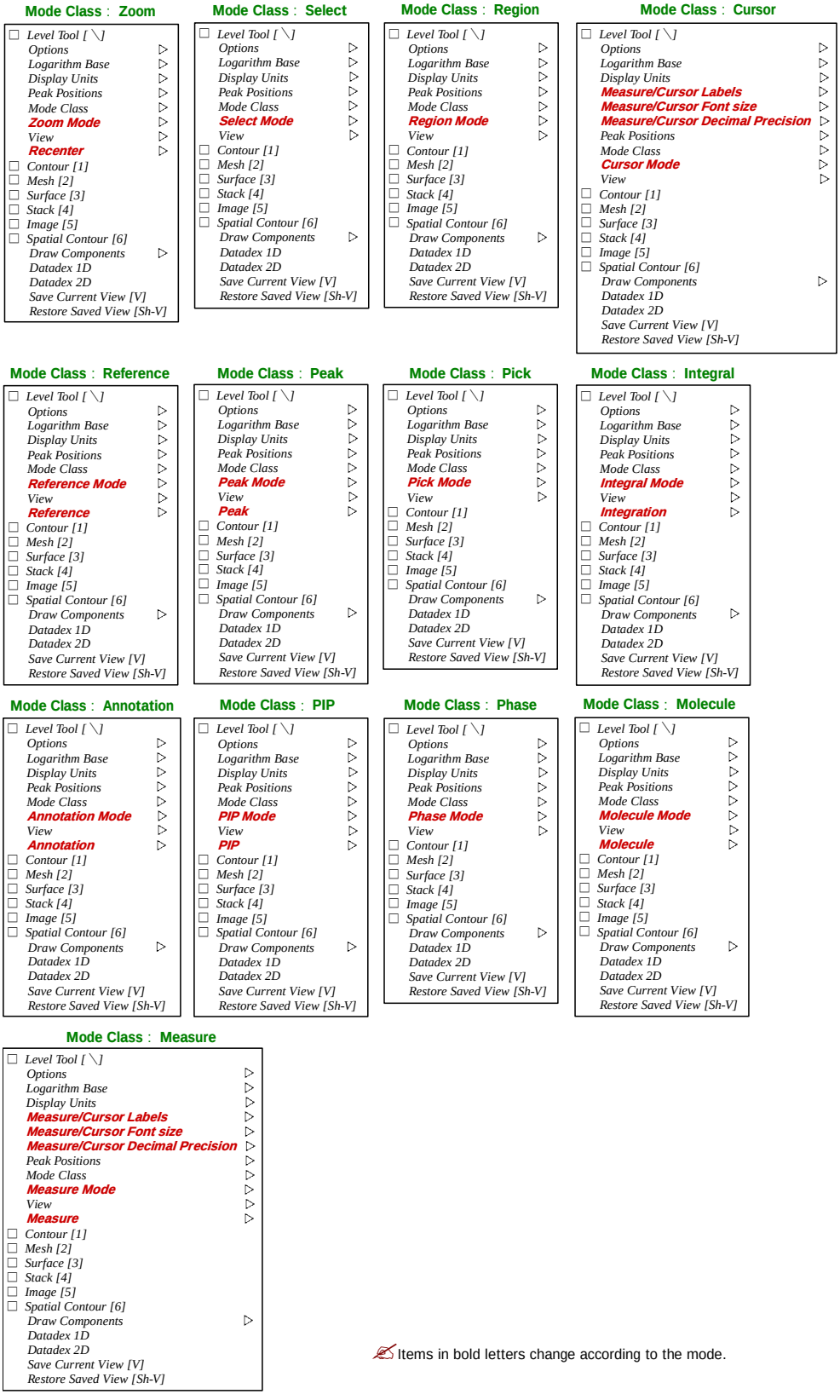
Pop-up menu for every Mode Class setting

The pop-up menu changes with the setting of **Mode Class** (Fig. 10.6).



Items in bold letters change according to the mode.

Fig. 10.6 Pop-up menu when the cursor tool is not displayed

Menu item

Item	Explanation	Display of item
Level Tool [\ ]	Displays the level tool.	All modes
Options	Sets the display item.	
Logarithm Base	Changes a unit for logarithm display.	
Display Units	Changes a unit of X axis.	
Measure/Cursor Labels	Changes the setting item for **Cursor** and **Measure.**	**Measure** **Cursor** mode
Measure/Cursor Font Size	Changes the font size for displaying **Cursor** and **Measure.**	
Measure/Cursor Decimal Precision	Changes the position of decimal points for displaying **Cursor** and **Measure**.	
Color of Selected Object	Changes the color of the selected text.	**Annotation mode** (when text appears)
Font of Selected Text	Changes the font of the selected text.	
Size of Selected Text	Changes the font size of the selected text.	
Attribute of Selected Text	Changes the character style of the selected text.	
Outline of Selected Text	Changes the outline of the selected text.	
Rotation of Selected Text	Changes the direction of the selected text.	
Peak Positions	Changes the display position of the peak values.	All modes
Mode Class	Changes cursor.	
Zoom Mode	Changes the setting items in the **Zoom** mode.	**Zoom** mode
Select Mode	Changes the setting items in the **Select** mode.	**Select** mode
Region Mode	Changes the setting items in the **Region** mode.	**Region** mode
Cursor Mode	Changes the setting items in the **Cursor** mode.	**Cursor** mode
Reference Mode	Changes the setting items in the **Reference** mode.	**Reference** mode
Peak Mode	Changes the setting items in the **Peak** mode.	**Peak** mode
Pick Mode	Changes the setting items in the **Pick** mode.	**Pick** mode
Integral Mode	Changes the setting items in the **Integral** mode.	**Integral** mode
Annotation Mode	Changes various setting items in **Annotation** mode.	**Annotation** mode.
PIP Mode	Changes the setting items in the **PIP** mode.	**PIP** mode.
Phase Mode	Changes various setting items in **Phase** mode.	**Phase** mode.
Molecule Mode	Changes the setting items in the **Molecule** mode.	**Molecule** mode
Measure Mode	Changes the setting items in the **Measure** mode.	**Measure** mode
View	Expands, reduces or resets for display.	All modes
Reference	Changes the settings for **Reference.**	**Reference** mode
Peak	Changes the settings for **Peak.**	**Peak** mode
Integration]	Changes the settings for **Integration**.	**Integration** mode

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Item	Explanation	Display of item
Annotation	Changes note set in **Annotation** mode.	**Annotation** mode
PIP	Changes the settings for **PIP.**	**PIP** mode
Recenter]	Changes the settings for **Zoom**.	**Zoom** mode
Molecule	Changes the settings for **Molecule**.	**Molecule** mode
Measure	Changes the settings for Measure.	**Measure** mode
Contour [1]	Performs contour plot display.	All modes
Mesh [2]	Performs mesh display.	
Surface [3]	Performs surface display.	
Stack [4]	Performs stack display.	
Image [5]	Performs image display.	
Spatial Contour [6]	Performs three-dimensional display.	
Draw Components	Selects component that you want to display.	
Datadex 1D	Sets slice display of 1D data.	
Datadex 2D	While displaying Datadex 1D, return it to 2D data.	
Save Current View [V]	Saves the currently displayed range.	
Restore Saved View [Sh-V]	Returns to the original state.	

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10.2.2 When Cursor Tool is being Displayed

When the cursor tool was being displayed, if you click the right button of the mouse on the geometry of **Data Slate** that display 2D data or **2D Viewer** window, a pop-up menu as shown in Fig. 10.7 appears.

✍ The cursor tool can be displayed by clicking its tab button, or by right clicking-**Option–Display–Show Cursor Tool**.

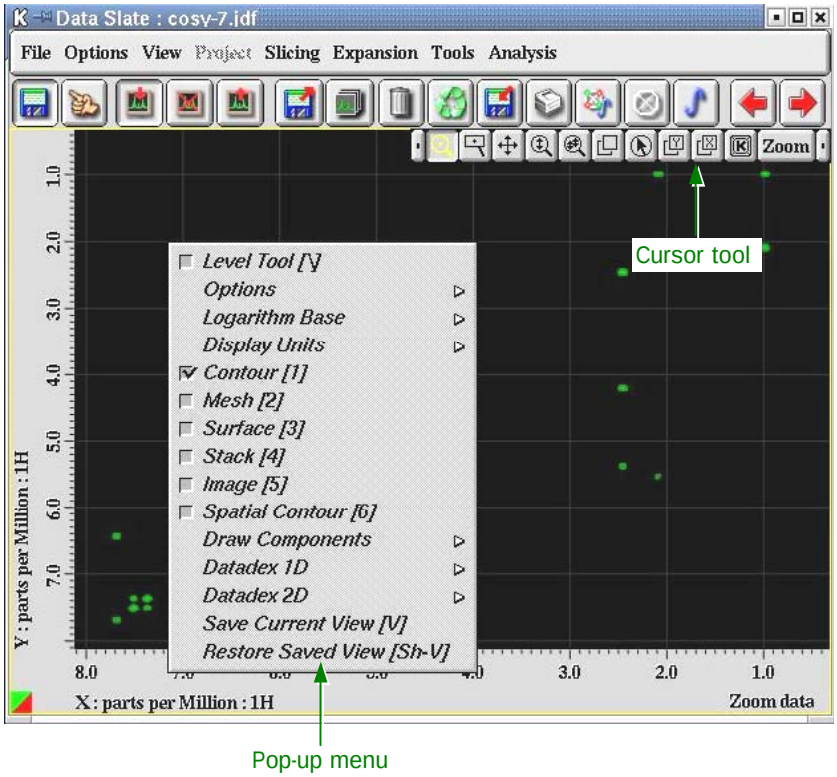

Fig. 10.7 The pop up menu in Zoom mode of the cursor tool

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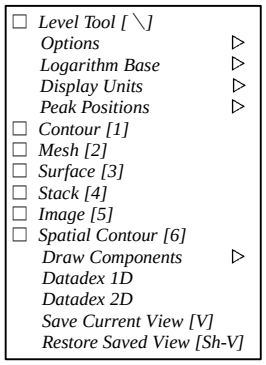
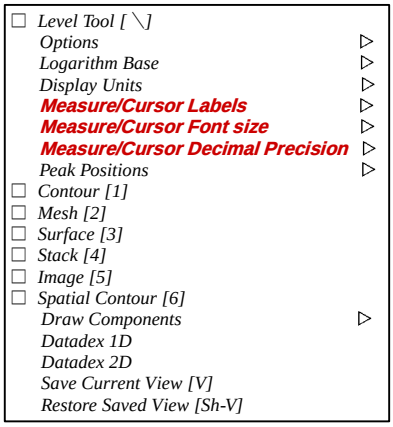
Pop-up menu for every display mode

When the cursor tool is **Measure** or **Cursor**, the pop-up menus differ from those in other Modes (Fig. 10.8).

Modes other than **Cursor** and **Measure** mode



In **Cursor** and **Measure** mode



Items in bold letters differ according to mode.

Fig. 10.8 Pop up menu when the cursor tool is being displayed

Menu items

Item	Explanation	Display
Level Tool [\ ]	Displays the level tool.	All modes
Options	Sets the display item.	
Logarithm Base	Changes the base in the logarithm display.	
Display Units	Changes the units of X and Y axis.	
Measure/Cursor Labels	Changes tables for **Cursor** and **Measure.**	**Measure** **Cursor** mode
Measure/Cursor Font Size	Changes font size for displaying **Cursor** and **Measure.**	
Measure/Cursor Decimal Precision	Changes the position of the decimal points for displaying Cursor and Measure.	
Color of Selected Object	Changes the color of the selected text.	**Annotation** mode (when text appears)
Font of Selected Text	Changes the font of the selected text.	
Size of Selected Text	Changes the font size of the selected text.	
Attribute of Selected Text	Changes the character style of the selected text.	
Outline of Selected Text	Changes the outline of the selected text.	
Rotation of Selected Text	Changes the direction of the selected text.	
Peak Positions	Changes the display position of the peak values.	All modes
Contour [1]	Performs contour plot display.	
Mesh [2]	Performs mesh display.	
Surface [3]	Performs surface display.	

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Item	Explanation	Display
Stack [4]	Performs stack display.	
Image [5]	Performs image display.	
Spatial Contour [6]	Performs three-dimensional display.	
Draw Components	Selects the component that you want to display.	
Datadex 1D	Sets slice display of 1D data.	
Datadex 2D	While Datadex 1D is displayed, returns it to 2D data.	
Save Current View [V]	Saves the current displayed range.	
Restore Saved View [Sh-V]	Returns to the original state.	

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10.2.3 Setting Each Item

The items on the display differ according to the display window, whether the cursor tool is displayed or hidden, and the present **Mode Class**.

■ Options

Item	Explanation	
Annotations[Alt-A]	Displays the notes which are set in the **Annotation** mode.	
Cursors[Alt-C]	Displays the cursor which is set in the **Cursor** mode.	
Measure[Sh-Alt-H]	Displays the measuring range which is set in the **Measure** mode.	
PiP Windows[Alt-W]	Displays the area of the PIP box which is set in the **PIP** mode on the spectrum.	
Regions[Alt-R]	Displays the area which is set in the **Region** mode.	
Integral	**Integrals [Alt-I]:**	Displays the integration curves which are set in the Integral mode.
	Integral Value [Alt-Q]:	Displays the integration curves.
Peak	**Center of Mass [Sh-Alt-W]:**	Calculates the center of the peak from the integration values and peak positions of two peaks, and display it.
	Peak Pick [Alt-P]:	Displays the peak information when in any mode other than Peak mode.
	Sequence [Alt-J]:	Displays the peak information which is set using spread sheet.
	Sequence Marker [Alt-M]:	Displays cursor on the peak which is displaying sequence.
Molecules	**Atom Numbers [Sh-Alt-A]:**	Numbers the skeleton of molecular structural formula which is displayed on the geometry.
	Atom Select Numbers [Sh-Alt-S]:	Numbers the selected skeleton.
	Atom Sequence [Sh-Alt-Q:	Displays the correction between the selected skeleton and peaks.
	Molecules [Sh-Alt-M]:	Displays the structure set in the molecular mode when displaying in any mode other than Molecular mode.
	Molecule Border [Sh-Alt-D]:	Displays a frame on the molecule.
	Molecule Title [Sh-Alt-T]:	Displays the title of molecule.
Data	**Data [Alt-D]:**	Displays data.
	Data Points [Alt-N]:	Displays the marker on each data points.
	Line Hinding [Alt-L]:	In the stack display, does not display the behind line of the stacking data.
	Statistics [Alt-T]:	Displays base level, noise level and threshold level of peak.

Item	Explanation	
	Center Contour Levels Around Baseplane Portion:	Corrects indication of contour plot based on the statistics which is set initially.
	Extra Data Color Solid:	Changes color when projection is performed on the surface of the cube in 3D display.
Display	**Grid [Alt-G]:**	Displays grid lines.
	Perspective [Alt-V]:	Changes display in 3D display.
	PIP Border [Alt-S]:	Display the frame of the PIP box.
	Plot Border [Sh-Alt-B]:	Display the frame of the Plot box.
	Plot Transparent [Alt-I]:	The part of the main spectrum which overlaps PIP box is also printed.
	Overlay Tabs [Sh-Alt-O]:	Displays the tab when writing overlaps.
	Scan to Threshold [Sh-Alt-R]:	When you want to search a slice data set automatically using threshold level, turn this on.
	Show Cursor Tool [Tab]:	Displays cursor tool.
File Information	**All Overlays [Alt-O]:**	In overwriting, displays file names of all spectra.
	Comment [Sh-Alt-O]:	Displays comment.
	File Name [Alt-F]:	Displays file name.
	Shadow Dimensions [Alt-B]:	Displays the position of a slice data set by point, percent or second.
Ruler	**X Rule [Alt-X]:**	Displays X axis.
	Y Ruler [Alt-Y]:	Displays Y axis.
	Z Ruler [Alt-Z]:	Displays Z axis.
	Logarithmic X Ruler [Sh-Alt-X]:	Displays X axis with logarithmic scaling.
	Logarithmic V Ruler [Sh-Alt-Y]:	Displays Y axis with logarithmic scaling.
	Show Number of Points [Sh-Alt-E]:	Displays point numbers on X axis.
	Show Ruler Type [Sh-Alt-G]:	Display ruler type on X axis.
	Display Clock Time X:	Displays X axis with human time.
	Display Clock Time Y:	Displays Y axis with human time.

Logarithm Base

Item	Explanation
X Ruler	Selects logarithm display from 2, e and 10.
Y Ruler	Selects logarithm display from 2, e and 10.

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Display Units

Item		Explanation	
X Ruler	**Hertz**	Displays X axis in Hertz.	
	ppm	Displays X axis in ppm.	
	Percent	Displays X axis in percent.	
	Points	Displays X axis in points.	
	Peak Units	**Hertz:**	Displays the chemical shift of picked peak in Hertz
		ppm:	Displays the chemical shift of picked peak in ppm
		Percent:	Displays the chemical shift of picked peak in percent
		Points:	Displays the chemical shift of picked peak in point
		Ruler Units:	Displays the chemical shift of picked peak in the same unit as that of X axis ruler.
	Measure/Cursor Units	**Hertz:**	Displays the unit of measuring range as Hertz.
		ppm:	Displays the unit of measuring range as points.
		Percent:	Displays the unit of measuring range as percent.
		Points:	Displays the unit of measuring range as points.
		Ruler Units:	Displays the unit of measuring range as the same unit as that of X axis ruler.
	Reset	Returns to the initial settings.	
	Cycle	Returns to the setting value one step prior to the present one.	
Y Ruler	**Hertz**	Displays Y axis in Hertz.	
	ppm	Displays Y axis in ppm.	
	Percent	Displays Y axis in percent.	
	Points	Displays Y axis in points.	
	Peak Units	**Hertz:**	Displays the chemical shift of picked peak in Hertz
		ppm:	Displays the chemical shift of picked peak in ppm
		Percent:	Displays the chemical shift of picked peak in percent
		Points:	Displays the chemical shift of picked peak in point
		Ruler Units:	Displays the chemical shift of picked peak in the same unit as that of Y axis ruler.
	Measure/Cursor Units	**Hertz:**	Displays the unit of measuring range as Hertz.
		ppm:	Displays the unit of measuring range as points.
		Percent:	Displays the unit of measuring range as percent.
		Points:	Displays the unit of measuring range as points.
		Ruler Units:	Displays the unit of measuring range by the same unit as that of Y axis ruler.
	Reset	Return to the initial setting.	
	Cycle	Return to the setting of before one step.	

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Peak positions

Item	Explanation
Show Peak Pos X	Displays position on X axis for selected peak.
Show Peak Pos Y	Displays position on Y axis for selected peak.
Show Peak Pos All	Displays position on X and Y axes for selected peak.
Show Peak Pos None	Does not display information for **Peak Positions.**

Measure/Cursor Labels

Item	Explanation
Show Measure X	Shows a length on the X axis for the selected measuring range.
Show Measure Y	Shows a length on the Y axis for the selected measuring range.
Show Measure Dist	Show a distance for the selected measuring range.
Show Measure All	Shows the length on the X and Y axes for the selected measuring range.
Show Measure None	Does not show the information for the measuring range.

Measure/Cursor Font Size

Item	Explanation
6～38	Changes the font size in a range from 6 to 38.
Default	Sets the font size to the default value.

Measure/Cursor Decimal Precision

Item	Explanation
1～12	Changes decimal places in a range 1 to 12 digits.
Default	Sets decimal places to the default value.

Draw Components

Item	Explanation
Draw Above Baseplane [Sh-1]	Displays the positive spectrum.
Draw Below Baseplane [Sh-2]	Displays the negative spectrum.

Datadex1D

Item	Explanation
X	Displays the slice data on X axis for the selected area in the Data Slate.
Y	Displays the slice data on Y axis for the selected area in the Data Slate.

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Datadex2D

Item	Explanation
X, Y	Returns to 2D display.

Mode Class

While the cursor tool is in the display, these modes can be changed on the cursor tool.

Item	Explanation
Zoom [F1]	Changes to **Zoom** mode.
Select [F2]	Changes to **Select** mode.
Region [F3]	Changes to **Region** mode.
Cursor [F4	Changes to **Cursor** mode.
Reference [F5]	Changes to **Reference** mode.
Peak [F6]	Changes to **Peak** mode.
Pick [F7]	Changes to **Pick** mode.
Integral [F8]	Changes to **Integral** mode.
Annotation [F9]	Changes to **Annotation** mode.
PiP [F10]	Changes to **PIP** mode.
Offset [F11	Changes to **Offse**t mode.
Molecule [F12]	Changes to **Molecule** mode.
Measure [Print Scrn]	Changes to **Measure** mode.

View

When the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Reset View [Home]	In expanded display, resets display area.
Reset All Dims [Sh-Ctl-Home]	When displaying a datadex, irrespective of selection geometry, resets the display range in both X and Y axes.
Unzoom [Bksp]	Undoes last zoom.
Cycle Slot + [PgUp]	When overwriting, selects spectra in the overwritten order.
Cycle Slot – [PgDw]	When overwriting, selects spectra in the overwritten inverse order.
Pan –Y [Dwn]	In expanded display, moves the spectrum downward.
Pan +Y [Up]	In expanded display, moves the spectrum upward.
Pan –X [Lft]	In expanded display, moves the spectrum leftward.
Pan +X [Rgt]	In expanded display, moves the spectrum rightward.
Expand –Y [Ctl-Dwn]	Reduces the display range along the Y axis.
Expand+Y [Ctl-Up]	Expands the display range along the Y axis.

Item	Explanation
Expand –X [Ctl-Lft]	Reduces the display range along the X axis.
Expand +X [Ctl-Rgt]	Expands the display range along the X axis.

Zoom Mode

Item	Explanation
Zoom data	Expands the surrounded area.
Pan data	Moves the spectrum in the vertical direction by the Y ruler and in the horizontal direction by the X ruler.
Expand data	Expands or reduces the spectrum in the vertical direction by the Y ruler and in the horizontal direction by the X ruler.
Apply Y gain	Expands and reduces the spectrum in the vertical direction.
Apply Y gain to all slots	Expands and reduces all the spectra overlapped in the vertical direction.
Offset overlay	Changes the display position in the vertical and horizontal direction for the selected spectrum from the overlapped spectra.
Cycle overlays	Displays the overlapped spectra.
Offset overlay in Y	While the spectra are displayed overlapping, moves the display position in the vertical direction.
Offset overlay in X	While the spectra are displayed overlapping, changes the display position in the horizontal direction.

Select Mode

Item	Explanation
Select geometry	Selects a geometry for operation.
Cycle overlays	When overwriting spectra in one geometry, selects the desired spectra.
Apply box analysis	When carrying out a certain operation on a limited area in one geometry, specifies the operation. Foe example, specify the range of application of **Zero Region** in the **2D Viewer** window.

Region Mode

Item	Explanation
Create region	Specifies a domain in **PIP** box creation. Perform **BOX** in the **Presentation Manager** window, and specify a domain in the **2D Phaser**.
Move/Resize region	Moves the PIP box, and changes its size. Moves the **BOX** and changes its size in **the Presentation Manager** window.
Delete region	Deletes **PIP** box. Delete BOX in the **Presentation Manager** window.

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Cursor Mode

Item	Explanation
Create cursor	Creates new cross cursor.
Move cursor	Moves the position of cross cursor.
Select cursor	Selects cross cursor.
Delete cursor	Deletes cross cursor.

Reference Mode

Item	explanation
Grab position for reference	Takes a frequency of a specified spectrum into the computer as a reference frequency.
Paste reference	Pastes a reference frequency on the specified position.
Paste reference to nearest peak	Pastes the reference to the nearest peak from the specified position.
Paste reference to all geometries	Pastes a reference on all the geometries of overlay display.
Cycle overlays	Click on the geometry of overlay display, selecting geometry move to the next.

Reference

While the cursor tool is in the display, these items are in the [K] key commands.

Item	Explanation
Round [R]	Display as integer.
Zero [Z]	If you select this command in **Paste reference** before pasting reference, the peak selected in **Paste reference** becomes zero.

Peak Mode

While the cursor tool is in the display, these items are in the [K] key commands.

Item	Explanation
Create peak	Sets up as a new peak to the peak top near the position selected.
Force create peak	Adds specified position as a peak.
Delete peak	Eliminates a peak.
Adjust peak threshold	Determines the detection peak level using the statistics set during peak picking.
Adjust noise threshold	Determines the noise level using the statistics set during peak picking.
Adjust baseplane / thresholds	Determines the base level using the statistics set during peak picking.
Select peaks	Selects the peaks set already.
Select more peaks	Selects more peaks when peaks are already selected.

Item	Explanation
Unselect peaks	Cancels peak selection.

Peak

While the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Select All [A]	Selects all peaks.
Unselect All [U]	Cancels the selection for selecting peaks.
Complement [C]	Switches the selected and unselected peaks.
Delete [Del]]	Eliminates the selected peaks.
Undelete [Ins]	Undoes delete.
Normalize [N]	Makes a reference of the integration value of a selected peak for the integration.
Group peaks [G]	Displays the center of selected signal group.
Meld peaks [M]	Displays the center of selected peak.
J Coupling [J]	Displays the coupling constant of selected peaks.
Sequence Search [S]	Searches the peak of the same value as that of the selected peak.
Center of Mass [W]	Displays the peak center using an integration value and peak position.
Recompute Stastics [R]	Recalculates statistics which are set automatically.

Pick Mode

Item	Explanation
Pick position	Reads peak position.
Copy position to buffer	Copies the read peak positions.
Copy position of nearest peak to buffer	Copies the position of the nearest peak from the specified position.
Set datadex slice point	Sets slice point for the extraction slice data to datadex.
Spear datadexed file	Displays peak position on the datadex.
Copy relative to center of ruler	Reads the distance between the selected peak and center of the spectrum, and places it to the cut and paste buffer in the **Delta Console** window.
Pick lower Contour Bound	Sets the lowest level of contour map using the projection or slice data.
Pick Upper Contour Bound	Sets the top level of contour map using the projection or slice data.
Pick Selected Contour Threshold	Sets the contour level which is selected using the **Level Tool** window in the projection or the slice data.

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Integral Mode

Item	Explanation
Create integral	Sets a new integration range.
Delete integral	Deletes an integration range.
Change slop of integral	Sets the slope in the integration range. Correct it by changing base point marker.
Adjust integral	Adjusts an integration range.
Split integral into two	Separates two parts at an arbitrary point which is selected on the integration curve.
Gain integrals in Y	Sets a length in the vertical direction in the integration range.
Change offset of integrals	Sets the position of integration curve in the spectrum.
Adjust peak threshold	Adjusts peak-detection level with the statistics set during peak picking.
Adjust noise threshold	Adjusts noise level with the statistics set during peak picking.
Adjust baseplane / threshold]	Adjusts base-line level with the statistics set during peak picking.
Select integrals	Selects the integration ranges which have been set.
Select more integrals	Selects more integration ranges after some integration ranges are already selected.
Unselect integrals	Cancels the selected integration ranges.

Integration

While the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Select All [A]	Selects all integration values.
Unselect All [U]	Cancels selection.
Complement [C]	Interchanges the selected and the unselected signals.
Delete [Del]	Deletes the selected integration ranges.
Undelete [Ins]	Undoes deletion of integral values.
Normalize [N]	Sets selected integration values to the values which are set in the **Set Integral Normalize**.
Gain Select [G]	Sets selected integration gain.
Recompute Statistics [R]	Recalculates statistics which are set automatically.

Annotation Mode

Item	Explanation
Create text annotation	Inputs text (comment) any where in the data-processing display area.
Edit text annotation	Changes the text.

Item	Explanation
Create Rectangle	Creates rectangle any where in the data processing display area.
Create Line	Creates a line on any place in the data processing display area.
Create Arrow	Creates an arrow any where in the data processing display area.
Create Double Arrow	Creates a two-side arrow any where in the data processing display area.
Move/Resize Annotation	Moves text and changes its size.
Delete annotation	Deletes text.
Select annotation	Selects text.
Add select annotation	Select more text while some text is already selected.
Unselect annotation	Cancels the selection.

Annotation

While the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Select All [A]	Selects all text.
Unselect All [U]	Cancels the selection of text.
Complement [C]	Selects everything except the currently selected text.
Delete [Del]	Deletes the selected text.
Cycle Font For Selected [Sh-Dwn]	Changes the font of the selected text in the order of the item in **Font of Selected Text**
Cycle Font For Selected [Sh-Up]	Changes the font of the selected text in the reverse order of the item in **Font of Selected Text**
Cycle Size For Selected [Ctl-Dwn]	Changes the font size of the selected text in the order of item in **Size of Selected Text**
Cycle Size For Selected [Ctl-Up]	Changes the font size of the selected text in the reverse order of the item in **Size of Selected Text**
Cycle Style Attribute For Selected [Alt-Dwn]	Changes the font style of the selected text in the order of the item in **Style of Selected Text**
Cycle Style Attribute For Selected [Alt-Up]	Changes the font style of the selected text in the reverse order of the item in **Style of Selected Text**

PIP Mode

Item	Explanation
Create PIP by zoom region	Creates a partial spectrum (PIP box) from a whole spectrum.
Move/Resize PIP zoom region	Moves the PIP box and changes its size.
Create PIP	Inserts a whole spectrum at any place in the processing data display area. The display area of the inserted spectrum can be changed by the **Zoom** mode.
Move/Resize PIP	Moves the PIP box created by **Create PIP**, and changes its size.

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Item	Explanation
Delete PIP	Deletes the PIP box.

PIP

While the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Prettify [P]	Arranges the **PIP** boxes.

Phase Mode

Item	Explanation
Adjust the Phase PP value	Adjusts the display phase parameter (PP).
Adjust the Phase P0 value	Corrects the zero order phase parameter (P0) .
Adjust the Phase P1 value	Corrects the first order phase parameter (P1).
Pick position	Reads a peak position.

Recenter

While the cursor tool is in the display, these are in the key commands.

項 目	説 明
Recenter [R]	In the overlay data, returns only the selected data to the original position.
Recenter Def [D]	In the overlay data, returns the display position of each data set to the positions in **File–Preference** of the **Delta Console** window.
Recenter All [A]	In the overlay data, returns to the original position.

Molecule Mode

Item	Explanation
Create Molecule window	Specifies a range when creating a **Molecule** window.
Move/Resize Molecule window	Moves the **Molecule** window.
Select Molecule window	Selects a **Molecule** window.
Delete Molecules window	Deletes a **Molecule** window.
Select Atom	Selects atoms of the **Molecule** window.
Select more peaks	Selects more peaks.
Unselect peaks	Cancels peak selection.

Molecules

While the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Attach to X [X]	Relates a displayed structural formula and the peaks of the spectrum.
Unattach to X [Sh-X]	Cancels relation between a displayed structural formula and the peaks.
Unselect Attched Atoms [T]	Cancels the selection of unrelated points of the structural formula.
Attach to Y[Y]	Relates a displayed structural formula and the peaks of the spectrum.
Unattach to Y [Sh-Y]	Cancels relation between a displayed structural formula and the peaks.
Unselect All Peaks [U]	Cancels selected points on structural formula related with all peaks.
Save Molecule File [S]	Saves the displayed structural formula.

Measure Mode

Item	Explanation
Create Measure	Sets the measuring range.
Create Measure in X	Specifies the measurement range in the X direction.
Create Measure in Y	Specifies the measurement range in the Y direction.
Resize Measure	Changes the measuring range.
Resize Measure in X	Changes the measurement range in the X direction.
Resize Measure in Y	Changes the measurement range in the Y direction.
Rotate Measure	Changes the direction of measuring range.
Select Measure Near Cursor	Selects the measuring range which is set.
Unselect Measure	Cancels the selected measuring range.
Delete Measure	Cancels the selected measuring range.

Measure

While the cursor tool is in the display, these items are in the key commands.

Item	Explanation
Unselect [U]	Releases the selected measuring range.
Delete Selected [D]	Deletes the selected measuring range.
Delete All [R]	Deletes all measuring range.
Display All [D]	Displays the measuring range and all information.

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